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INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY  
UNION INTERNATIONALE DE CHIMIE PURE ET APPLIQUÉE



# COMPTES RENDUS XXV CONFERENCE

CORTINA D'AMPEZZO

30 June—8 July 1969

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International Union of Pure and Applied Chemistry  
1970

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**COMPTES RENDUS  
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CORTINA D'AMPEZZO

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Prof. P. D. BARTLETT (President of IUPAC Organic Chemistry Division), Department of Chemistry, Harvard University, 12 Oxford Street, Cambridge, Massachusetts 02138 (USA)

Prof. P. W. WEST (President of IUPAC Analytical Chemistry Division), Coates Chemical Laboratories, Louisiana State University, Baton Rouge, Louisiana 70803 (USA)

## **Venezuela (1)**

Dr. G. CHUCHANI, Instituto Venezolano de Investigaciones Cientificas, Apartado 1827, Caracas (Venezuela)

## **Yugoslavia (2)**

Prof. M. L. MIHAJLOVIC, Marsala Tita 6/II, Beograd (Yugoslavia)



# **OFFICIAL DELEGATES OF ASSOCIATED ORGANIZATIONS AT XXV CONFERENCE**

## **European Federation of Chemical Engineering**

Dr. D. BEHRENS, DECHEMA, Postfach 970146, D-6000 Frankfurt/Main 97  
(Germany)

## **International Committee for Electrochemical Thermo- dynamics and Kinetics**

Prof. J. KORYTA, J. Heyrovský Polarographic Institute, Czechoslovak  
Academy of Sciences, Opletalova 25, Praha 2 (Czechoslovakia)

## **International Federation of Clinical Chemistry**

Prof. M. RUBIN, Department of Biochemistry, School of Medicine, George-  
town University Hospital, 3800 Reservoir Road NW, Washington, DC  
20007 (USA)

# **AGENDA FOR XXV COUNCIL MEETING**

**Cortina d'Ampezzo—5th and 7th July 1969**

1. Finalization of Agenda
2. Approval of Minutes of XXIVth Council Meeting
3. Announcement of Nominations for Officers and Bureau Members
4. Announcement of Time of Elections
5. Statutory Report of President on State of the Union
6. Biennial Report of Treasurer
7. Report of Finance Committee
8. Applications for Change of Category
9. Budget for 1970 and Tentative Budget for 1971
10. Dues Structure
11. Fixing Annual Dues for 1970 and 1971
12. Report of Committee on Teaching of Chemistry
13. Report on Publications
14. Reports of Division Presidents and Clinical Chemistry Section
15. Adoption of Final Nomenclature Rules
16. Bureau Proposals for New Units
17. Ratification of Decisions taken by Bureau and Executive Committee since XXIVth Conference
18. Elections
19. Date and Place of XXVIIth Conference and XXIVth Congress
20. Any Other Business

# REPORT OF PRESIDENT ON STATE OF THE UNION

IUPAC 1967-1969

IUPAC has entered the second half-century of its existence during last year (1968). Within the past 50 years our Union has acquired great success in its activities. It may be stated with great satisfaction that IUPAC is now widely known, that its prestige and authority continuously increase, and that more and more countries become its members. Yet much remains to be done in order that all the activities of IUPAC are consistent with its aims, and that the situation becomes such that contacts of National Organizations with IUPAC be an indispensable condition for development of chemistry in any country.

Still greater activity of Divisions, Sections, and Commissions, strengthening of the existing and establishment of new contacts with National Organizations, more ready response to the requirements of industry would be necessary for this purpose. All this was emphasized before in the reports of IUPAC Presidents.

As far back as 1955 Prof. A. TISELIUS said 'I stressed the importance of a rationalization of our Commission work, which, after all, is the most essential part of our activities' and further on 'Many of our Commissions do very fine work and have justified their existence beyond any doubt. I am not so sure about certain others, however.' He also mentioned the desirability of establishing closer contacts with National Organizations on questions 'requiring collaboration between different nations' particularly in view of the 'great practical and industrial importance of chemistry'.

Prof. W. A. NOYES, Jr., also emphasized that wider activity of Divisions, Sections, and Commissions was necessary. He was explicit in defining the two main directions of contacts between IUPAC and all bodies interested in its activities. First 'drawing rules for nomenclature, symbols, values of constants, *etc.*' and second 'furnishing advice' to industry on questions on which IUPAC is a 'recognized authority'.

Lord TODD, in developing upon Prof. NOYES' ideas, has pointed, in particular, to the necessity of 'making our Division Committees more effective working bodies' . . . 'to fulfil our functions properly and to justify increasing support which we are now receiving'. Lord TODD thought that one of the ways towards it was the strengthening of the IUPAC Secretariat.

Lord TODD spoke of 'the astonishing increase in the influence of the Union during the past ten years' and was confident in IUPAC success, saying that 'the future of the Union is in our hands'.

Prof. W. KLEMM drew attention to the necessity of considerably greater activity in the field of applied chemistry.

He said that every second year the Bureau and Council should, in the light of the Division President's report, decide whether or not to continue a Commission, a rule that did not seem to be carefully observed. The Division Committees must have a great responsibility in this matter. In order to bring the Commission organization into harmony with the By-laws, to achieve greater efficiency, and to save money, Prof. KLEMM proposed that each Division Committee should consider thoroughly which Commissions are necessary for long-term work, which must be given a certain time to finish their work, and which should be dissolved. Since there were Commissions whose main purpose appeared to be the organization of symposia he doubted



that these should have as many as eight members for this purpose, though it certainly is a very useful and necessary task.

The ideas put forward by Prof. KLEMM were repeated and defined again in my memorandum submitted to the IUPAC Council in Prague. This memorandum was approved by the Executive Committee, the Bureau, the Division Presidents, and the Council. I firmly believe that sooner or later it will be put into practice. I also hope that great help will be received in this respect from our Secretariat.

It may be stated now that we have come much closer to realization of the above-mentioned conditions which we all consider as indispensable for the prosperity of our Union. Great progress has occurred during the two past years.

This may be seen, in particular, from the strengthening of contacts between IUPAC and industry. In the past, close contacts with chemical industry were, in fact, realized only by the Division of Applied Chemistry, whereas now the Analytical Chemistry Division is also involved in it. The very productive activities of the two Divisions in the work under contract with CE yielded results of general interest.

This is how the work was started. At first Prof. R. TRUHAUT and the Secretary General convinced the authorities of the European Community in Brussels to enter into a contract with IUPAC for the establishment of analytical methods for determination of criteria of purity for food additives. In fact, control of the human environment by analytical methods must be done on a truly world-wide scale and IUPAC is the body for achieving this task. Up to this time, 47 analytical methods have been collected, carefully checked, and delivered in a draft form to Brussels. This is the first step of IUPAC activity in an advisory capacity to international organizations. Parallel to the work under contract with CE, cooperation continues with the specialized United Nations agencies.

The necessity of considerably greater activity in the field of applied chemistry has been stressed by Prof. KLEMM in his presidential report. In particular he has expressed the wish to have within the Union a strong Division concerned with theoretical and practical problems of macromolecular chemistry. A relevant decision was made at the Conference in 1967. A Macromolecular Division was created on the basis of the Commission of Macromolecular Chemistry of the Physical Chemistry Division and the Section on Plastics and High Polymers of the Applied Chemistry Division. The latter two units have been correspondingly dissolved.

The Division started its work immediately and elected Prof. O. WICHTERLE as its President. This new Division, from the very beginning, has cooperated closely with chemical industry, and now successfully combines academic science and its application to practice. Great efforts are being made to elaborate clear rules for nomenclature in this particularly complicated field. It is important that special attention be paid to the necessity of adapting nomenclature to retrieval by machines. The latter problem was tentatively considered by the Executive Committee this February and a final decision was postponed until this Conference.

You know that on the initiative of the Secretary General and through the far-sighted action of Lord TODD, the IUPAC Company Associates Plan was accepted by Council in 1965. I am happy to say that during the period of my Presidency this plan developed beyond any prognostics. Quite recently, at the beginning of 1969, our colleague and friend, Prof. S. SHIBATA, informed us that 17 chemical companies (with a total of 21 units) from Japan had applied for the status of IUPAC Company Associate.

This plan gives IUPAC a great opportunity of closer cooperation with chemical industry, and our Divisions, Sections, and Commissions will be in a position to draw on the expertise of a great mass of chemists working in chemical industry.

With the same purpose Lord TODD proposed to organize a symposium on *Modern Chemistry in Industry* that was convened in Eastbourne (UK), in March 1968. During this symposium the representatives of chemical industry came into closer contact with those of academic science. There was an exchange of information on mutual interests, requirements, and wishes of both sides.

Certain steps were taken in the direction of establishing closer relations with National Adhering Organizations. I have talked of it at the Prague Conference in 1967. I stressed, in particular, the necessity of having a reasonably higher number of Associate Members and National Representatives in order that the activities of relevant Divisions, Sections, and Commissions be brought nearer to the requirements of National Organizations. In this connection and also with a view to strengthening IUPAC contacts with industry, the National Committee of Soviet Chemists has informed several Ministries of the USSR concerned with chemistry about IUPAC activities and has asked them what would be their requirements from IUPAC. Some of the answers received were sent to the IUPAC Secretariat and also to the relevant Division Presidents, Dr. W. GALLAY and Prof. P. W. WEST. The accompanying letter of the National Committee of Soviet Chemists contained a suggestion that it might be expedient to ask all National Adhering Organizations what is the extent of the interest of their national bodies in IUPAC and what would be their wishes. I firmly believe that without the interest of national bodies in IUPAC activities and direct perceptible benefit to them, proper appreciation of our Union and its high prestige would hardly be possible.

Our Commissions and Sections have done very fine and important work during the past two years and I appreciate it greatly, but I shall not enumerate here the achievements of these main working Units of IUPAC, since you will hear of them from the Division Presidents.

Now about the structure of our Union. It underwent some essential changes during the term of my office. First of all a new IUPAC Secretariat has been set up in 1968. Let me remind you of some stages in its formation.

As mentioned before, the necessity of having a strong Secretariat was pointed out by Lord TODD in his presidential report. He stressed its importance in connection with the increased activities and scope of the IUPAC programme, and considered it a means for increasing the efficiency of Division Committees. The problem became particularly acute after Mr. C. SAVAGE left for a job in the Swiss industry. An *ad hoc* Committee, consisting of Prof. KLEMM, Lord TODD, Dr. D. C. MARTIN, and Dr. R. MORE, was appointed at the LVIIIth meeting of the Executive Committee in order to propose candidates for Executive Secretary.

The *ad hoc* Committee proposals were discussed at the LXth meeting of the Executive Committee in February 1968. Dr. M. WILLIAMS was appointed Executive Secretary. It was resolved that for two years the IUPAC Secretariat will be located in Oxford. Clerical help to Divisions was taken as one of the most important tasks of the new Secretariat. I believe that the latter will also be of great help in putting into practice all the decisions made by IUPAC officials.

A Macromolecular Division about which I spoke earlier was created by decision of the Prague Conference.

Clinical chemistry has become now of most important help in diagnostics,



due to the development of new analytical methods, apparatus, and tools. IUPAC, recognizing its impact on humanity all over the world and wishing to improve the recognition and the standing of clinical chemistry, has created in 1967 a very active Section of Clinical Chemistry. Also, the International Federation of Clinical Chemistry has been granted the status of an Associated Organization of IUPAC. The clinical chemists under the umbrella of IUPAC are standardizing their analytical methods, fixing units and measurements, stimulating education and training of clinical chemists, and organizing congresses and symposia on clinical chemistry.

At present the Clinical Chemistry Section consists of three Commissions: on Quantities and Units, on Teaching of Clinical Chemistry, and on Automation.

In the same year of 1967 the IUPAC Council decided to dissolve the Biological Division on account of the existence of IUB. The Joint IUPAC-IUB Nomenclature Commission was transferred to the Organic Chemistry Division. This Commission has been extremely active.

Two *ad hoc* Committees—on Plasma Chemistry and on Medicinal Chemistry—were appointed by decision of the Bureau. They will submit their considerations as to the desired nature and form of IUPAC activities in these fields. I would only add that medicinal chemistry had and continues to have the most remarkable impact on human and animal health, and I presume that Council will agree to creating a new Section of Medicinal Chemistry attached directly to the Bureau.

The Bureau and Executive Committee have also considered the proposals stated in my second memorandum about including the problem of tabulation of kinetic constants in the IUPAC programme and increasing the IUPAC activities in the field of catalysis.

The question of kinetic constants is not new for our Union. It was in the programme of the Commission headed by Prof. K. F. BONHOEFFER. This Commission was dissolved after his death.

The importance of tabulation of kinetic constants has immeasurably increased at present. When I initially raised this problem, it was not then clear whether the ICSU Committee on Data for Science and Technology (CODATA) would consider it a part of its work. It was resolved at the CODATA meeting at the beginning of this year that a kinetic group be organized inside CODATA, and now the question arises only as to what will be the part of IUPAC in the work of this group. I think that for the beginning the best decision would be that IUPAC undertakes the work on electrochemical kinetics, including it into the programme of our Electrochemistry Commission.

As to catalysis, a consultation with the President of the Council of the International Congress on Catalysis, Prof. J. H. DE BOER, took place and the IUPAC Executive Committee decided that Prof. J. Th. G. OVERBEEK, Chairman of our Commission on Colloid and Surface Chemistry, will be IUPAC's representative to the Council of the Congress. This is the first move towards establishing closer contact between IUPAC and the Congress, which was on the agenda for a long time.

These are the changes in the structure of IUPAC that have either taken place or are envisaged.

One of the tasks of IUPAC is the study of various problems connected with chemical education and the working out of relevant recommendations. As a report on this topic will be presented at this Conference, I shall restrict myself to very short information.

Chemical education has been stimulated by the IUPAC Committee on Teaching of Chemistry, with Sir RONALD NYHOLM as its Chairman. Sir



RONALD is at present the President of The Chemical Society in London. Because of his heavy load of work, he was forced to resign from the Chairmanship of the Teaching Committee, and the Executive Committee has approved Prof. R. W. PARRY as the new Chairman. I am convinced that Council will ratify this decision.

I shall not discuss here IUPAC publication matters, guided with such skill and cleverness by Sir HAROLD THOMPSON and Prof. B. C. L. WEEDON. Sir HAROLD will present a report himself.

Also I shall not speak much about our budget and financial affairs which will be discussed in the reports of our Honorary Treasurer and the Chairman of the Finance Committee. We all know the high quality of their work. The state of our finances shows that our Union is prospering and has grown to a strong position.

Naturally, the IUPAC budget increases in parallel with the activities of our Sections and Commissions. The budget of even several years ago no longer suits the aims and practice of today. Consequently, we must attach great importance to the motion of the USA Delegation directed to an increase in the subscriptions of countries with developed chemical science and industry, and I hope that the discussion of this problem which is included on the Council meeting agenda will yield an appropriate solution to it.

We must not forget that there is another condition of our Union's prosperity. I mean the extent of expenses. For instance, we must avoid meetings of low efficiency, and the Divisions, Sections, and Commissions must always take into account the expediency and necessity of any expense.

In conclusion I would like, first of all, to express on behalf of the IUPAC Council and as IUPAC President, our thanks to the Italian Research Council, to the Italian Tourist Company, and personally to Prof. G. SARTORI for their kind hospitality and all the arrangements they made. I am confident that the work of the Conference will have great success and will add to the prestige of our Union.

I wish to thank the Bureau, the Executive Committee Members, and the staff of our Secretariat for their active and fruitful work and for the cooperation and friendly help they gave me. I express my sincerest gratitude to Dr. MORF whose help was particularly valuable and necessary. I also wish to thank most earnestly the Divisions, Sections, and Commissions for their important work.

Dr. A. L. G. REES becomes IUPAC President today. It was obvious long ago that Dr. REES, a fine scientist and excellent organizer, always paying such vivid interest to IUPAC affairs, will make a perfect President. I think that we can promise Dr. REES to assist him in any respect that he will need, and wish him the greatest success.

We are all looking forward, with great expectation, to the forthcoming International Congress in Australia. The incoming President, Dr. REES, is the President of the Congress, which is one of the best guarantees for its success. Dr. J. R. PRICE and his distinguished Organizing Committee have worked very hard to guarantee the great success of the Congress.

V. N. KONDRATIEV  
President

# BIENNIAL REPORT OF TREASURER FOR 1967-8

## I. Introduction

The International Union of Pure and Applied Chemistry not only continues to fulfil the functions which its founding fathers had in mind, but it is seeing new areas of service and is expanding the scope of its activities. Under a contract with UNESCO, it is conducting studies in the field of chemical education and helping to guide the progress of chemistry teaching in the developing countries; and under a contract with the European Community, (CE), it is assembling a list of proved, standard methods of analysis, particularly for foodstuffs that are articles of international trade. At the same time, it is trying to strengthen the programme which its Divisions and Sections have traditionally carried on, and the sponsorship of symposia for which it is so widely known. It must not only assume new functions in response to demands; it must anticipate those demands and meet them as they arise. To do so, and simultaneously, to exert a stronger influence in its traditional roles, will require an ever increasing budget, as well as a larger group of volunteer workers. As was mentioned in the Biennial Report for 1965-66, IUPAC should be an umbrella organization, covering all aspects and all branches of international chemistry. We cannot allow its work to be fragmented.

## 2. Income

There has been no large increase in income from dues during the biennium, for no new bodies have joined IUPAC, and only four countries have gone into higher categories—Canada, France, Japan, and Italy, all of which now pay \$5,000 per year instead of \$2,600. There seems little likelihood that income from dues will increase very much under the present dues structure. Several methods of increasing dues income have been proposed, the most attractive being a plan which would base the dues of each National Body on the chemical turnover of its country. A plan of this sort, which was briefly mentioned in our report for 1965-66, was formally proposed at the Conference in Prague, but was found unsatisfactory in some respects. It has been modified considerably in the hope of eliminating the undesirable features, and is now being discussed by the National Bodies. It may need further modification. While it may seem easy to devise such a plan, it is actually very difficult, for economic systems differ a great deal in different countries. It is hoped, however, that a satisfactory plan will soon be adopted.

The Company Associates Plan has developed slowly but well, and it is still our hope that it will bring in \$40,000 in 1969. The Company Associates Plan is much more than a source of revenue—it furnishes a much needed link between IUPAC and chemical industry—a link which we have tried to strengthen for several years. Currently, there are Company Associates in only ten countries, which is about one-fourth of the countries represented in IUPAC. Let me urge all of the Adhering Bodies to solicit Company Associates, and to maintain close contact with them. The National Body may, if it wishes, retain up to 5% of the receipts of the Company Associates in its country, utilizing this money solely to further the Company Associates programme—*e.g.*, it may hold meetings with the Company Associates to discuss IUPAC programmes or it may distribute literature describing the work of IUPAC.

The four Swiss chemical companies, which have so generously supported the office of the Secretary General, have now found it necessary to discontinue that support. This is, of course, regrettable from IUPAC's point of view, but we are grateful for the help which they gave us over a period of more than twelve years. It was only with this help that IUPAC prospered and grew to its present strong position. Happily, IUPAC has now reached a place where it can carry on without this help.

Financial help comes to IUPAC from many sources—most of its Officers and those of its Divisions, Sections, and Commissions are able to call on their employers for stenographic help and the use of office equipment. Some of these contributions are large, and some are small. In total, they add up to many thousands of dollars each year. We are grateful, too, to the Adhering Bodies in Canada, France, and Italy, and to the United States National Science Foundation and the Academy of Sciences of USSR, who paid part or all of the expenses of Titular Members from their respective countries to the XXIVth Conference in Prague in 1967. We wish to express our thanks to the Science Council of Japan, which voluntarily limited the number of Japanese Titular Members who attended the Conference in Prague. We hope that they will continue such generosity in future years. Because of the generosity of these Adhering Bodies, the travel expense charged to IUPAC in 1967 was actually less than that charged in 1968, even though the former was a Conference year.

Our journal, *Pure and Applied Chemistry*, continues to improve in quality, although it still does not attract a large subscription list. All Company Associates receive it as part of our service to them, and this doubtless cuts down on the number of libraries and companies that would subscribe to it otherwise. We hope that the growth of the Company Associates Plan will more than offset this factor. There are, of course, royalties from *Pure and Applied Chemistry*, but they are relatively small. A somewhat larger income results from the sale of reprints and separates.

The contracts with UNESCO and the European Community do not result in a net financial gain to IUPAC, for we spend on their projects all of the money which is received. This is permissible, for through its work with these agencies, IUPAC is rendering a real service and is increasing its prestige among chemical organizations.

We must again express our thanks to the Schweizerische Bankgesellschaft which, for many years, has handled our accounts. Originally, the Bank rendered this great service at no cost to IUPAC. In more recent years, we have suggested that we pay the Bank a nominal fee. This has been increased this year, but certainly does not pay for the excellent and generous service which the Bank gives us. We thank particularly Mr. G. HANSELMANN, who handled this work for several years, Mr. H. BAUMANN, who has now taken this work over, and Dr. J. RAKOWSKY, who has worked indefatigably in our behalf.

### 3. Expenses

With the establishment of the IUPAC Secretariat, which is now fully operative in Oxford, IUPAC assumed a major increase in expenses. The staff includes the Executive Secretary, an Assistant Secretary, and three stenographers. The Secretariat is set up to aid the Officers and the Commissions by handling all administrative details. It is hoped that since the Secretary



General will thus be relieved of most of such administrative work, he can devote his time more fully to planning and to matters of policy.

The largest single expense item in budget is, of course, the item for travel. This increases steadily, both because prices continue to go up and because IUPAC is electing more and more Titular Members from Asia and other lands distant from Europe and North America. Although this is expensive, it is a desirable trend—we look forward to the day when IUPAC will have very greatly increased activity in Africa and South America, too. IUPAC continues to pay travel and subsistence expenses for its members who travel on IUPAC business, and it is hoped that this practice, initiated in 1963, can be continued indefinitely. It has increased the expense of meetings (the attendance of Titular Members at Prague was about 90%), but it has greatly improved the operation of the Commissions and of IUPAC.

The exact figures relating to the Income and Expenditure Accounts, and the Balance Sheet, can be seen in the report of the Auditors, which is in the following pages.

J. C. BAILAR, JR.  
Treasurer

Zürich, 29th January 1969  
Löwenstrasse 56

*To the Executive Committee  
International Union of Pure and Applied Chemistry  
Zürich—Switzerland*

## **AUDITORS' REPORT ON ACCOUNTS**

**Years ended 31st December 1967 and 1968**

We have examined the balance sheets of the International Union of Pure and Applied Chemistry as at 31st December 1967 and 1968 and the related statements of profit and loss for the two years then ended. Our examination was made in accordance with generally accepted auditing standards and accordingly included such tests of the accounting records and such other auditing procedures as we considered necessary in the circumstances.

In our opinion, the enclosed balance sheets and the statements of income and expenditure together with the return of supplementary information present fairly the financial position of the International Union of Pure and Applied Chemistry at 31st December 1967 and 1968 and the results of its operations for the two years then ended, in conformity with generally accepted accounting principles.

*Neutra Auditing Inc.*  
(J. Lauber) (H. Heller)

# COMPARATIVE BALANCE SHEETS

(Expressed in

## Assets

	1967	1968
Cash in Bank .. .. .	19,402.65	21,915.31
Bankers Acceptances (Commercial Bills) .. .. .	91,000.—	91,000.—
Bullion Account .. .. .	14,176.45	14,176.45
Marketable Securities—at cost (Approximate Market Value, as at December 1968, \$275,105.—) .. .. .	146,111.19	196,440.50
Other Assets .. .. .	3,658.90	6,249.50

US-\$ 274,349.19 329,781.76

*Note:* Subscriptions outstanding as at  
31st December 1968, aggregating .. .. . US-\$ 3,350.—

# COMPARATIVE STATEMENT OF INCOME AND

(Expressed in

## Income

	1967		1968	
<i>Subscriptions</i>				
Current Year .. .. .	88,885.55		95,244.37	
Previous Years .. .. .	5,648.50		14,716.57	
Voluntary Contributions .. .. .	12,280.—*		—.—	
Voluntary Contribution from Germany .. .. .	10,000.—		—.—	
Company Associates .. .. .	30,557.48	147,371.53	31,870.64	141,831.58
<i>Interest and Dividends Earned</i> .. .. .	7,278.79		12,143.12	
<i>Less:</i> Transfer to Reserve a/c .. .. .	7,278.79	—.—	12,143.12	—.—
<i>Sales of Publications</i> .. .. .		179.64		66.57
<i>Royalties from Butterworths</i> .. .. .	7,406.50		6,440.—	
<i>Less:</i> Transfer to Reserve a/c .. .. .	7,406.50	—.—	6,440.—	—.—
<i>Other Income</i>				
Contract Teaching of Chem- istry (UNESCO Special Subvention) .. .. .	1,500.—		3,000.—	
CE Brussels .. .. .	5,051.69		2,025.52	
Reimbursement of Contribu- tion 1966 and 1967 (non paid) to ICSU .. .. .	1,707.48	8,259.17	1,793.51	6,819.03
<i>Exchange Differences</i> .. .. .		—.—		225.05
		<u>155,810.34</u>		<u>148,942.23</u>

## UNESCO/ICSU GRANT ACCOUNTS

Subvention collected during Year .. .. .	14,000.—	14,000.—
Special Grant from ICSU for CE Contract .. .. .	8,000.—	—.—
	US-\$ <u>177,810.34</u>	US-\$ <u>162,942.23</u>

\*Of which Germany \$5,000.— and UK £2,600 (\$7,280.—)



# AS AT 31 DECEMBER 1967 AND 1968

US-Dollars)

## Liabilities and Net Worth

	1967	1968
Accrued Liabilities .. ..	14,853.95	2,300.—
Net Worth:		
Capital Account .. ..	102,139.36	107,926.36
Reserve .. ..	95,533.45	183,489.16
	<u>197,672.81</u>	<u>291,415.52</u>
Plus: Excess of Income over Expenditure for the 12 Months ended 31st December ..	61,822.43	36,066.24
	259,495.24	327,481.76
US-\$	<u>274,349.19</u>	<u>329,781.76</u>

# EXPENDITURES—YEARS ENDED 31 DECEMBER 1967 AND 1968

US-Dollars)

## Expenditure

	1967	1968
<i>Office Expenses</i>		
(Salaries, Printing, Stationery and Miscellaneous)		
General Office and Sections ..	24,320.26	8,511.67
Office of Secretary General (Zürich) .. ..	—.—	10,623.06
IUPAC Secretariat (Oxford) ..	—.—	21,723.17
	<u>24,320.26</u>	<u>40,857.90</u>
<i>Travel and Subsistence Expenses</i> (incl. UNESCO a/c) .. ..	18,282.71	58,541.26
<i>Special Account</i> (Prague Conference) .. ..	38,486.08	—.—
<i>Contract CE/ICSU</i> .. ..	7,571.21	—.—
<i>Contribution to Symposia</i> .. ..	—.—	4,000.—
<i>Publications</i> .. ..	10,587.90	14,043.77
	<u>99,248.16</u>	<u>117,442.93</u>
Less: Subvention collected from UNESCO/ICSU .. ..	14,000.—	14,000.—
CE Special Grant .. ..	<u>8,000.—</u>	<u>—.—</u>
	77,248.16	103,442.93
<i>Other Expenses</i>		
Contract Teaching of Chemistry .. ..	3,031.38	4,127.96
Bank Charges .. ..	523.30	705.12
Subscription to ICSU .. ..	1,793.51	1,890.68
Audit and Accounting Charges .. ..	1,273.14	2,709.30
Voluntary Contribution from Germany in favour of 4 Chemical Companies in Basle .. ..	<u>10,000.—</u>	<u>—.—</u>
	16,621.33	9,433.06
<i>Exchange Differences</i> .. ..	118.42	—.—
<i>Excess of Income over Expenditure</i> (for the 12 months ended 31st December) .. ..	61,822.43	36,066.24
	<u>155,810.34</u>	<u>148,942.23</u>
<b>UNESCO/ICSU GRANT ACCOUNTS</b>		
Total Expenditures .. ..	15,577.80	28,979.15
Less: To Debit of IUPAC Funds .. ..	<u>1,577.80</u>	<u>14,979.15</u>
	14,000.—	14,000.—
Expenditures CE-a/c .. ..	7,571.21	—.—
Plus: Unexpended Balance .. ..	428.79	8,000.—
US-\$	<u>177,810.34</u>	<u>US-\$ 162,942.23</u>

## INCOME OF IUPAC FROM NATIONAL ADHERING ORGANIZATIONS IN 1968

Country				Category				Annual Subscription \$
Argentina	..	..	..	C	..	..	..	450
Australia	..	..	..	A1	..	..	..	2,600
Austria	..	..	..	C	..	..	..	450
Belgium	..	..	..	A1	..	..	..	2,600
Brazil	..	..	..	B1	..	..	..	800
Bulgaria	..	..	..	C	..	..	..	450
Canada	..	..	..	A2	..	..	..	5,000
Colombia	..	..	..	C	..	..	..	450
Cuba	..	..	..	D	..	..	..	100
Czechoslovakia	..	..	..	B1	..	..	..	800
Denmark	..	..	..	A1	..	..	..	2,600
Finland	..	..	..	B1	..	..	..	800
France	..	..	..	A1	..	..	..	5,000
Germany	..	..	..	A3	..	..	..	10,000
Greece	..	..	..	D	..	..	..	100
Hungary	..	..	..	C	..	..	..	450
India	..	..	..	B2	..	..	..	1,600
Ireland	..	..	..	D	..	..	..	100
Israel	..	..	..	B1	..	..	..	800
Italy	..	..	..	A2	..	..	..	5,000
Japan	..	..	..	A1	..	..	..	2,600
Mexico	..	..	..	C	..	..	..	450
Netherlands	..	..	..	A1	..	..	..	2,600
New Zealand	..	..	..	C	..	..	..	450
Nigeria	..	..	..	D	..	..	..	100
Norway	..	..	..	B1	..	..	..	800
Poland	..	..	..	B1	..	..	..	800
Portugal	..	..	..	C	..	..	..	450
Republic of China	..	..	..	B1	..	..	..	800
Republic of Korea	..	..	..	C	..	..	..	450
Republic of South Africa	..	..	..	B1	..	..	..	800
Republic of Vietnam	..	..	..	C	..	..	..	450
Romania	..	..	..	C	..	..	..	450
Spain	..	..	..	B1	..	..	..	800
Sweden	..	..	..	A2	..	..	..	5,000
Switzerland	..	..	..	A1	..	..	..	2,600
Turkey	..	..	..	D	..	..	..	100
United Arab Republic	..	..	..	C	..	..	..	450
United Kingdom	..	..	..	A3	..	..	..	10,000
USA	..	..	..	A4	..	..	..	25,000
USSR	..	..	..	A1	..	..	..	2,600
Venezuela	..	..	..	D	..	..	..	100
Yugoslavia	..	..	..	C	..	..	..	450

# IUPAC FINANCE COMMITTEE

## Report of Meeting held in Zürich on 21 January 1969

The Finance Committee met in the premises of the Schweizerische Bankgesellschaft at Zürich, Switzerland. All Members of the Committee were present and Dr. R. MORF (*ex-officio*). They were joined by Mr. H. FISCHER of the Bank for discussion of investments, and by Messrs. G. HANSELMANN and H. BAUMANN for lunch.

### 1. Agenda

The agenda as prepared by Dr. MORF was amended, and is reflected in these minutes as it was revised.

### 2. Minutes

Minutes of the last meeting of the Finance Committee (22nd February 1968, in Zürich) were approved.

It was noted that the Executive Committee had considered and taken action on certain recommendations made by the Finance Committee (Executive Committee Minutes 372 and 376, LXth Meeting, London).

### 3. Transfer of Funds to Reserves

Pursuant to previous recommendations of the Finance Committee, \$10,000 had been transferred annually to reserves. The Committee believed that reserves were now sufficient in relation to annual expenditures, and it recommended that the mandatory \$10,000 annual transfers be terminated, effective with the current fiscal year.

### 4. Terms of Reference of Committee

Discussion of terms of reference of the Finance Committee led to the conclusion that those terms (*Comptes Rendus XXII Conference*, page 158, cipher 7. Decision of Council in London, July 1963, that: 'in place of the present arrangements for *ad hoc* Finance Committees a standing Finance Committee, of not more than five members, be set up to advise the Bureau and Executive.') are adequately defined for the present, but that one change is desirable.

The Committee discusses investments with the IUPAC banker at its meetings in Zürich. Decisions made should be implemented promptly, because of possible changes in the securities markets. Also, changes in investments may need to be made between meetings of the Committee. In such cases, agreement may be reached by correspondence. The Bureau, the Executive Committee, and the Treasurer do not take part in the detailed review of the investments, and do not always act promptly on Finance Committee recommendations.



The Finance Committee recommended that the Finance Committee be given executive authority with respect to selection, purchases, and sales of securities held by IUPAC, provided that the Schweizerische Bankgesellschaft, as the IUPAC banker, concurs in the decisions of the Committee.

The Finance Committee also recommended that its Chairman or delegate should be present at Bureau and Executive Committee meetings when financial matters are being considered.

### **5. Categories of Membership**

The Finance Committee had previously recommended revision of the membership categories for the purpose of establishing a more rational relationship between the size of the chemical industry of a country and the amount of its annual subvention to IUPAC. At the Council meeting in Prague, the USA Delegation made a specific proposal to implement the Finance Committee's recommendation, and the matter was later referred to an *ad hoc* committee for further study. The report of the *ad hoc* committee was reviewed by the Finance Committee. The Finance Committee considered the proposal of the *ad hoc* committee a very good compromise of the many conflicting factors involved in making such a change in membership categories. The Finance Committee recommended that preparations be made for final action on this matter at the coming Council meeting in Cortina d'Ampezzo.

### **6. Biennial Accounts**

The Committee examined the biennial accounts, and found them in good order.

### **7. Company Associates**

The Committee noted that income from the Company Associates Plan is now between one-third and one-fourth of total annual income. The Committee resolved to express thanks to Prof. S. SHIBATA and Dr. K. HOSHINO for their work in securing a large number of supporting industrial organizations in Japan.

### **8. Investments**

The Committee reviewed the investments and noted with satisfaction that the market value of the securities had greatly increased. It was concluded that capital gains should not be taken at this time, because of the lack of any better securities for replacement. On the other hand a number of small investments showing losses should be sold, as they probably will not improve in the foreseeable future, and the funds can be put into securities with better prospects. Detailed selections of securities for sale and purchase were made with the advice of the Bank, and the Treasurer was informed, for his confirmation of action to be taken.

## **9. Banker**

The Schweizerische Bankgesellschaft had long been the IUPAC banker, accountant, and auditor, in part because of the previous location of the Secretariat. In view of present circumstances, the relationship with the Schweizerische Bankgesellschaft should be put on a somewhat more formal basis. The Finance Committee recommended that the Secretary General writes a letter to the Schweizerische Bankgesellschaft

- (1) asking it to continue as the IUPAC banker, and
- (2) asking for an estimate of its expenses as IUPAC banker, so that these may be paid by IUPAC.

The amount now paid by IUPAC is unrealistic in relation to the Bank's costs, and it cannot be expected to continue indefinitely its gratuitous services.

## **10. Budget**

The Committee reviewed the Budget for the coming fiscal year. It recommended that the Executive Committee gives favourable consideration to increasing the maximum subvention given to an IUPAC-sponsored symposium, in order to make such sponsorship more meaningful. The Committee suggested an increase from the present limit of \$2,000 to a limit of \$6,000.

P. M. ARNOLD  
Chairman, Finance Committee

# COMMITTEE ON TEACHING OF CHEMISTRY

## Report to Council

(Item 12, Council Meetings, 5th and 7th July 1969)

### I. Introduction

The Committee on Teaching of Chemistry was founded in 1964 with Sir RONALD NYHOLM (UK) as its first Chairman. Sir RONALD relinquished his duties as Chairman in April 1969, and his successor is Prof. R. W. PARRY (USA). We are pleased that Sir RONALD has agreed to remain as a member of the Committee, and we wish to express our thanks to him for his distinguished leadership during the critical first five years of Committee activity. In addition, two members, Prof. W. A. NOYES, Jr. (USA) and Prof. O. A. REUTOV (USSR), retired from the Committee this year. We thank them for their service. Prof. A. F. PLATÉ (USSR) has been appointed to replace Prof. REUTOV.

As noted by Sir RONALD in his report to Council in 1967, the rate of development of Committee programmes is still restricted by our limited financial resources. We are grateful to IUPAC for part of our funds and to UNESCO for help with specified projects; however, additional resources are sorely needed. We are currently exploring the possibility of obtaining assistance from several private philanthropic organizations which have a strong interest in education.

### 2. Existing Programmes

During the first five-year period the Committee was actively concerned with three principal topics: (A) Examinations, (B) In-service Training of Teachers, (C) Supply of Chemistry Students for University-level Courses. The current status of each project is summarized below.

#### A. Examinations

An earlier Committee report on examinations (The Mathews Report—*The Effect of Examinations in Determining Chemistry Curricula*) has been followed up by an IUPAC-sponsored *International Workshop on Evaluation and Assessment* held in Ceylon in August 1968. The report of this highly successful workshop will be available during 1969. Major financial support was provided by UNESCO, CREDO (UK) and the Ceylon Ministry of Education.

#### B. In-service Training of Chemistry Teachers

A Committee report on this topic was published in *Information Bulletin* No. 31 (March 1968). At its April 1969 meeting the Committee was concerned with methods for implementing the recommendations contained in this report. One of the most urgent recommendations was presented to Council in the 1967 report of Sir RONALD NYHOLM. We quote 'That in-service training for teachers should be introduced to provide for a minimum of four weeks, preferably three months, retraining every five years for all teachers of chemistry in all countries at the secondary or high school level.' We would like to bring this recommendation to the attention of all IUPAC National Adhering



Organizations, Ministries of Education, and other national organizations concerned with the supply and training of chemistry teachers.

In a broader sense, the Committee felt that better communication with educationalists and policy makers in different countries is mandatory if the programmes of the Committee are to have the impact desired. Accordingly we recommend that:

- (1) The IUPAC Secretariat continues to expand its much appreciated efforts in the dissemination of information on the activities of IUPAC in the field of chemical education.
- (2) A system of *Correspondents* to the Committee be established. Such Correspondents would be appointed by, and work through their National Adhering Organizations. Each Correspondent would receive agendas, reports of meetings, project reports, and other appropriate documents. In turn comments, suggestions, advice, and informal reports would be given to the Committee by each Correspondent.
- (3) Notes and articles on the Committee's work should be sent to chemical education journals for publication. Members of the Committee will assume this responsibility.

### C. *Supply of Chemists for the Future*

The Berry Report on *The Supply of Chemistry Students for Tertiary Education* is available in draft form and was considered by the Committee at its last meeting. Preliminary data indicate an alarming decline in the number of students beginning the study of chemistry. The observation seems to be world wide. We believe that a problem of this gravity demands serious and careful study. Factual data rather than opinions are needed. A proposal calling for a detailed and documented study of enrolment in chemistry programmes is being prepared. This proposal will be presented to various philanthropic organizations in the hope that funds for a full-time study can be obtained.

### D. *Meetings and Publications on Chemical Education*

- (1) *Meetings.* The National Research Council of Italy and the IUPAC Committee on Teaching of Chemistry are jointly sponsoring a symposium on *University Chemical Education*. The meeting will be held in Frascati, Italy, on 16-19th October, 1969. An outstanding programme is anticipated.

The Committee has endorsed and will participate in an *International Symposium on Chemical Education* to be held during July 1970 in Colorado, USA. This meeting is being organized by the Division of Chemical Education of the American Chemical Society and celebrates its 50th anniversary as a Division of the American Chemical Society. A conference on *Chemical Education* is to be held in Sao Paulo, Brazil, in September 1970. The organizing committee has requested official IUPAC sponsorship.

Relations with the ICSU Committee on Science Teaching have also been maintained. Several members of the IUPAC Committee took part in an ICSU-sponsored conference on *The Integration of Science Teaching* which was held in Varna, Bulgaria, during September 1968.

- (2) *Publications*. Collaboration with UNESCO has been maintained and we are currently engaged in the compilation, under contract, of a *Guidebook on Chemistry Teaching at the Secondary School Level*. We are also advising on the form and content of *A Survey of University Chemistry Teaching* which will be compiled by UNESCO during 1970-71.

### 3. Future Programmes

Preliminary investigations have been started on new programmes. If preliminary data justify additional work, a more complete study of each topic will be undertaken. The topics are: (1) Supply and Training of Chemical Technicians, (2) Programmes for the Retraining of Professional Chemists Whose Training has become Obsolete, (3) A Comparative Review of the Various New Teaching Programmes in Secondary School Chemistry.

Views of Council delegates on any phase of this report will be welcomed.

Finally, speaking for the Committee, I would like to thank Mr. D. G. CHISMAN for his outstanding service as Secretary. Also deserving commendation are Dr. M. WILLIAMS, Mr. R. J. M. RATCLIFFE, and members of the IUPAC Secretariat staff for doing an excellent job in assisting with our work.

R. W. PARRY  
Chairman, Committee on Teaching of Chemistry

# I. PHYSICAL CHEMISTRY DIVISION

## Report of President

(Item 14, Council Meetings, 5th and 7th July 1969)

### I.1. Physicochemical Symbols, Terminology, and Units Commission

The new version of the *Manual of Symbols and Terminology for Physicochemical Quantities and Units*, including all the Prague revisions, was submitted to the Commission Members in August 1967, and published in *Information Bulletin* No. 32 (August 1968). A large number of detailed comments and suggestions have arrived from other Commissions. A two-day meeting of the Commission was held at Exeter on 19-20th December, 1968, to deal with the suggestions received. The Commission will meet for the first three days of the Conference at Cortina to consider any suggestions arriving after December 1968 and to finalize the Manual for submission to the Division for its approval.

*Suggestions for the Future.* The Commission should turn its attention away from basic principles, because the revised Manual will probably last for several years (up to ten), and aim at adding *Appendices* relating to special fields of physical chemistry, e.g., *Standard Thermodynamic Functions*, *Electrochemical Quantities*, *Spectroscopic Quantities*, *Quantities of Surface and Colloid Chemistry*.

### I.2. Thermodynamics and Thermochemistry Commission

1. Arrangements are complete for the *Ist International Conference on Calorimetry and Thermodynamics*, to be held in Warsaw, 31st August-4th September, 1969. This Conference is sponsored by the Polish Academy of Sciences, in honour of the late W. SWIETOSLAWSKI. The request for sponsorship by IUPAC was not granted.

2. *Bulletin of Thermodynamics and Thermochemistry*. No. 11 was published in June 1968 (457 pp.).

3. The first issue of the *Journal of Chemical Thermodynamics* (Academic Press) was published in January 1969. The Bureau has resolved that this journal must be published on a basis entirely independent of IUPAC and of Commission I.2.

4. An *ad hoc* Committee, consisting of Dr. C. W. BECKETT (USA), Chairman, Dr. L. DEFFET (Belgium) and Dr. V. V. SYTCHEV (USSR), has been appointed to study the question of *Plasma Chemistry* and the Committee is to report to the Bureau at Cortina. This Committee is already working by correspondence but arrangements are in hand to try and hold a meeting at Cortina.

5. Members of the Commission, and of the Thermodynamic Tables Project, contributed to the *Ist Codata Conference*, held at Arnoldsheim, Frankfurt, in July 1968.

6. The first publication of the Thermodynamic Tables Project (on properties of carbon dioxide) is nearly ready for publication.



### 1.3. Electrochemistry Commission

1. *Electrochemical Thermodynamics*. Prof. G. MILLAZZO will submit a collection of data—based on *critical* compilations from the relevant literature—encompassing electrode potentials, Gibbs free energies, heats, and entropies. Coverage includes organic media and fused salt solvents. This project will be judiciously coordinated with complementary activities of Commission V.5 (see 5 below). (It is anticipated that definitive tabulations will evolve from this long-range effort. The emerging data will be submitted for publication in due course, and thus be made available to the scientific community at large.)

2. *Electrochemical Kinetics*. Commission I.3 will consider for final approval a set of guidelines—developed by Prof. H. FISCHER, Prof. J. JORDAN, Dr. E. LEVART, Dr. R. TAMAMUSHI, and Prof. N. TANAKA—for the design of mechanistically significant electrochemical experimentation. Publication is envisaged through appropriate channels. Dr. TAMAMUSHI and Prof. TANAKA will submit a questionnaire intended to solicit significant information from laboratories engaged in fundamental research on electrode kinetics. The Tamamushi-Tanaka tabulation of kinetic parameters, published in 1964, will be updated by these authors under the auspices of Commission I.3.

3. *Nomenclature*. In response to a suggestion emanating from the Chairman of Commission I.1, Commission I.3 will discuss definite proposals for an *Electrochemical Appendix* to the *Manual of Physicochemical Symbols and Terminology*. Prof. J. KORYTA has circulated relevant material and comments, submitted by a group of distinguished electrochemists which includes several members of Commission I.3. The consensus of opinion of Commission I.3 on this matter, crystallized in Cortina d'Ampezzo, will be shared with Commission V.5. The Chairmen and Secretaries of Commissions I.3 and V.5 may subsequently submit joint recommendations for appropriate action by Commission I.1.

4. *Symposium on Non-Aqueous Electrochemistry*. A programme has been scheduled for July 1970 in Paris, co-sponsored by Commissions I.3 and V.5. Seven plenary lectures and thirty papers will be presented. Profs. I. M. KOLTHOFF and G. CHARLOT are Honorary Chairman and Local Arrangements Chairman, respectively. Dr. J. BADOZ is Executive Chairman, assisted by an *ad hoc* committee made up of the Parisian members of Commissions I.3 and V.5. Sponsorship by IUPAC has been granted.

5. *Liaison with Other IUPAC Commissions on Matters of Complementary Interest*. Several inter-Commission meetings have been planned for Cortina d'Ampezzo, between Chairmen, Secretaries, and Members of Commissions I.1, I.3, and V.5.

6. *Inter-biennial Commission Meetings*. The following synopsis lists meetings which have taken place since the XXIVth IUPAC Conference (Prague, 1967) and/or have been tentatively scheduled between the XXVth (Cortina, 1969) and forthcoming XXVIth (Washington, DC, 1971) Conferences:

March 1968, Paris—Chairmen and Secretaries of Commissions I.3 and V.5  
September 1968, Detroit—Titular and Associate Members of Commission I.3 and the Chairman of Commission V.5

Between September 1969 and August 1970 (time, place and possible participation of Commission V.5 to be agreed later)—Representatives of Commissions I.1 and I.3

July 1970, Paris—Titular and Associate Members of Commission I.3.

#### **I.4. Data and Standards Commission**

1. The good office of Dr. R. MORF, Secretary General, was utilized to request of the National Adhering Organizations a list of the substances certified with respect to a particular physical property by the national standardizing laboratories of the world. A standard substance is interpreted as one which reproduces a certified value of a physical property within a given accuracy, and may be applied to the following types of measurement:

- (i) calibration and standardization of instruments
- (ii) proof of measurement accuracy by a given method
- (iii) transfer of measured quantities between laboratories
- (iv) comparison of measurements by different laboratories.

Numerous replies have been received and the results are being collated.

2. Under date of 29th December, 1967, Commission Member Prof. H. KIENITZ proposed the establishment of a Task Group to search for and evaluate reference substances whose physical constants are established with sufficient accuracy for the intended use. Correspondence within the Commission revealed a majority in favour of participating, so on 26th June, 1968, a Physical Property Task Group (PPTG) was established with Prof. KIENITZ as Chairman. The Task Group has been asked to report to the Bureau at Cortina.

3. During 8, 9 and 10th July, 1968, an editorial panel consisting of Drs. L. A. K. STAVELEY (Chairman), E. F. G. HERINGTON, W. M. SMIT and D. R. STULL met at Oxford, UK, to review and consider the manuscript chapters of a monograph entitled *The Characterization of Chemical Purity*. The monograph currently has the following status: 9 typed chapters in final form, 1 chapter just arrived, 2 chapters outstanding.

#### **I.5. Molecular Structure and Spectroscopy Commission**

The Commission has held two meetings; the first was at Madrid (9-10th September, 1967) in association with the *IXth European Congress on Molecular Spectroscopy*, and the second (20th August, 1968) was at a *Gordon Conference on Infrared Spectroscopy* at Meriden, New Hampshire, USA. The comments here will be restricted to matters on which material progress has been made during the past year.

1. *Specifications for Evaluated Infrared Spectra*. About 100,000 infrared spectra are listed in five major collections. A master index, administered in the USA, is currently being reorganized for computer-based search.

Because the filed spectra are of varied quality and structural reliability, there is a need for internationally acceptable specifications. The draft set of specifications has been approved by the Titular Members of the Commission (postal vote) and published as tentative recommendations in *Information Bulletin* No. 34 (April 1969). The Commission will also circulate them to

other chemical spectroscopists. It hopes that a final version can be prepared at the XXVth Conference for formal approval by the Division.

2. *The SI Unit System.* Because spectroscopy is an interdisciplinary science, the ICSU Joint Commission on Spectroscopy ensures that actions taken in one of the disciplines concerned (astronomy, physics, chemistry) are compatible with practice in the others.

The spectroscopic sections of the draft version of the *Manual of Physico-chemical Symbols and Terminology* have been discussed by Commission I.5 and reviewed by Commission I.1, then referred to the ICSU Joint Commission. Any outstanding ambiguities ought to be thus resolved, so that Commission I.5 could be able to support acceptance of the Manual. Approval by the Division could then occur at the XXVth Conference.

The Commission's concern has been increased by statements in the general scientific literature which indicate that the Editorial Boards of a number of chemistry journals are proposing to institute precipitate and compulsory adoption of the SI System before IUPAC has had the opportunity to clarify ambiguities. It recognizes that editorial action of this kind is a separate matter from the formal approval of the SI System by IUPAC, but it is unfortunate that this situation has arisen to confuse the issue.

3. *Infrared Wavenumber Calibration below 600 cm<sup>-1</sup>.* Sub-Commission I.5.1 is now prepared to extend calibration tables at least to 200 cm<sup>-1</sup>. Additional measurements are currently made in several laboratories (Dr. R. N. JONES, Prof. R. C. LORD, Prof. F. A. MILLER). The results will probably be reported at the XXVth Conference.

4. *Laser Raman Spectroscopy.* Prof. E. R. LIPPINCOTT is heading a US National Bureau of Standards Committee, which is assessing the standards for measurements of Raman intensities and presentation of Raman spectra. A report will be ready for the next technical session.

5. *Specifications for the Presentation of NMR Spectra.* Initial difficulties have been cleared up. Prof. N. SHEPPARD and the British NMR Discussion Group will probably submit the draft recommendations at or before the next Conference.

6. *Spanish-English Version of the 'Multilingual Dictionary of Important Terms in Molecular Spectroscopy'.* Has now been published in the Instituto de Optica.

## **I.6. Colloid and Surface Chemistry Commission**

At the Prague meeting, the Commission decided to concentrate on the following activities in the near future:

1. Finalize a tentative nomenclature proposal for publication in the *Information Bulletin*.
2. Organize a symposium on surface area determination.
3. Initiate steps to promote the teaching of colloid and surface chemistry.



The present status of each of these activities is summarised below.

1. *Nomenclature.* The *Proposals for Terminology and Symbols in Colloid and Surface Chemistry*, drafted June 1967, are being modified by Prof. J. Th. G. OVERBEEK to accommodate comments received from Members of the Commission, from Commission I.1 and from ISO/TC91 and the Comité international des Dérivés tensioactifs. An additional section to this draft which will deal specifically with physical adsorption at the gas/solid interface is being prepared by Prof. D. H. EVERETT on the basis of an earlier draft prepared by a sub-committee. Another additional section dealing with chemisorption and catalysis, on which no agreement has been reached yet within the Commission, will not be included. The nomenclature proposals for terminology and symbols in colloid and surface chemistry should reach the position at Cortina when permission for tentative publication can be requested.

2. *Symposium on Surface Area Determination.* This is jointly sponsored by IUPAC and the British Society of Chemical Industry, and will be held at the University in Bristol, England, 17-19th July, 1969. The symposium is intended to survey the field and to guide efforts of ISO and national standards organizations in standardizing area determination methods. Representatives of these organizations have been invited to attend and participate in the symposium.

3. *Teaching of Colloid and Surface Chemistry.* The Commission proposes to create a work-textbook, to be used in conjunction with standard physical chemistry courses, which would offer attractive theoretical and practical exercises in colloid and surface chemistry, as a specific illustration of the physical chemistry course. This approach will be fully discussed at the next Commission meeting.

### **I.7. ICSU Joint Commission on Applied Radioactivity (JCAR)**

Since 1966 the Commission has only been functioning through correspondence. Its work has been confined to co-sponsoring international meetings. For 1968 the following meetings have been co-sponsored:

April 1-5	Symposium on the Effect of Radiation on Cellular Proliferation and Differentiation (Co-sponsored by IAEA and JCAR)	Monte Carlo (Monaco)
August 7-13	International Symposium on Meteorite Research (Organized by IAEA, in co-operation with UNESCO, JCAR, IAU, IUGS, IAGG and Meteoritic Society)	Vienna (Austria)
November 1-8	Symposium on the Use of Nuclear Techniques in the Prospecting and Development of Mineral Resources	Buenos Aires (Argentina)

Permission to disband this Commission is likely to be sought at Cortina.

H. W. MELVILLE  
President, Physical Chemistry Division

## II. INORGANIC CHEMISTRY DIVISION

### Report of President

(Item 14, Council Meetings, 5th and 7th July 1969)

#### II.1. Commission: Poids Atomiques

Conformément à la méthode de travail adoptée par la Commission depuis plusieurs années, chacun de ses membres a poursuivi sa tâche d'information dans son domaine propre. C'est au cours de la réunion de la Commission prévue à Cortina que seront confrontées ces informations, et c'est seulement à l'issue de cette réunion qu'un rapport pourra être établi à l'intention du conseil. Parmi les points faisant l'objet d'une attention particulière, figurent les variations d'abondance isotopique résultant

- (1) de la diversité des sources naturelles
- (2) de la mise en circuit commercial de produits ayant subi une séparation isotopique

#### II.2. Commission: Nomenclature

La Commission a maintenant terminé la révision des règles de 1957 et espère qu'une nouvelle édition pourra être publiée après la Conférence de Cortina. Ce chapitre 7 (composés de coordination) a été notablement étendu et a déjà été publié sous cette nouvelle forme à titre provisoire. La Commission désire inclure dans ce chapitre les règles décrivant la configuration absolue des composés de coordination optiquement actifs et les règles de Nomenclature des complexes cyclopentadienyles qui ont été approuvées à la réunion de Copenhague (Août 1968). En outre, les chapitres sur les phases cristallines de composition variable et sur les iso- et hétéropolyanions ont été modifiés et étendus.

La Commission prépare enfin les règles de nomenclature pour les composés du bore, les composés organosiliciques et organophosphoriques. Ces documents doivent être publiés en collaboration avec la Commission de Nomenclature en Chimie Organique.

#### II.3. Commission: Hautes Températures et Réfractaires

##### 1. *Etalons secondaires de température (S. J. Schneider, coordinateur)*

Le travail entrepris sur la détermination de la température de fusion de l'alumine a été complété par les 8 groupes de travail représentant 7 pays.

Les lignes directrices étaient les suivantes:

- (1) Utilisation d'un même matériau: alumine pure (>99,9 %) fournie par le Dr. FOEX (France), après fusion au four solaire.
- (2) Emploi des creusets de tungstène
- (3) Liberté totale du choix des conditions: moyen de chauffage, atmosphère, méthode statique ou dynamique.
  - 4 groupes ont utilisé l'analyse thermique
  - 3 groupes ont utilisé les méthodes d'observation directe
  - 1 groupe a utilisé l'observation après trempe d'échantillons chauffés à une température donnée et trempés.

La principale difficulté, quelle que soit la méthode, est la mesure de la température.

Les résultats sont les suivants:

2043°C (1 groupe); 2045°C (1 groupe); 2054°C (3 groupes);  
2055°C (2 groupes); 2073°C (1 groupe).

Les valeurs moyennes sont les suivantes:

- de tous les résultats: 2054°C (déviati on standard: 9°C)
- en excluant la valeur 2073°C: 2051°C (déviati on standard: 5,2°C)
- en excluant les 2 valeurs extrêmes: 2053°C (déviati on standard: 3,9°C)

La température de fusion de l'alumine semble donc comprise entre 2051°C et 2053°C. Puisque les erreurs sont généralement par défaut, la valeur 2053°C est la plus probable.

La Commission recommande à l'Advisory Committee on Thermometry de faire adopter la température de fusion de l'alumine comme étalon secondaire de l'International Practical Temperature Scale.

Le groupe de travail envisage maintenant les déterminations sur d'autres matériaux:  $Y_2O_3$  ( $\sim 2400^\circ C$ ), et peut être  $ZrO_2$  ( $\sim 2800^\circ C$ ). Quatre des membres ont déjà donné leur accord.

## 2. *Etalons de pression de vapeur (R. C. Paule, coordinateur)*

Le programme a été établi de la manière suivante:

- 5 éléments: Cd, Ag, Au, Pt, W
- Domaine de pression:  $10^{-3}$  à  $10^{-8}$  atm
- Domaine de température: 100—3000°C
- Méthodes: Langmuir, Knudsen, spectromètre de masse

30 laboratoires effectuent les mesures.

Le travail a d'abord été effectué sur l'or et commence maintenant sur le cadmium et l'argent.

Les valeurs les plus probables des pressions d'équilibre de l'or sont indiquées de 1300°K à 1200°K.

## 3. *Bibliographies (J. J. Diamond, coordinateur)*

Plusieurs modifications importantes sont intervenues.

- les bibliographies séparées sur les états condensés et les gaz ont été réunies en une seule.
- les recherches au-dessous de 1000°C ne sont plus envisagées.
- la distribution gratuite est devenue impossible. Les exemplaires sont maintenant vendus au prix d'impression par l' US Government Printing Office.

## 4. *Autres Activités*

Deux domaines qui semblent nécessiter une coopération internationale, sont envisagés:

- recherches sur le carbone (coordination des mesures et de la nomenclature)
- spectrométrie de masse.

J. BÉNARD  
President, Inorganic Chemistry Division



### III. ORGANIC CHEMISTRY DIVISION

#### Report of President

(Item 14, Council Meetings, 5th and 7th July 1969)

The Organic Chemistry Division is aware of having a large and diverse public to serve. To form an estimate of its size, we recently obtained figures from the Chemical Societies in Japan, Australia, Canada, India, Czechoslovakia, France, and the United States of America as to the distribution of their chemists among the principal fields. (A number of other societies reported that such information was not available from their records since they do not have a sectional organization plan.) In the countries in question organic chemistry is the *principal interest* of 28 %, 16 %, 'about 50 %', 16-25 %, 'about 44 %', and 10.8 %, respectively, of the member chemists. In the American Chemical Society, the Divisions *concerned with* organic chemistry are those of Food Chemistry, Biochemistry, Carbohydrate, Cellulose, Fuel, Medicinal Chemistry, Microbial Chemistry and Technology, Organic Chemistry, Organic Coatings and Plastics, Petroleum, Polymer, and Rubber Chemistry. Their total membership is 22,786 out of a total divisional membership of 47,916, or 47.5 % of the whole. By similar methods of counting, only the Applied Chemistry Division has a larger constituency.

In its recent meetings the Organic Chemistry Division Committee has given careful thought to the question of how best to serve its large international community in addition to its traditional and continuing work on the standardization of nomenclature. We are of the opinion that our most important work is the promotion of international contacts among research chemists by organizing symposia and conferences in active fields. We considered and rejected the idea of delegating this work to a special Commission, choosing instead to make the planning of symposia our chief item of business at and between our biennial meetings. In the course of this work we have sponsored some very successful symposia, thanks to a good deal of understanding and cooperation on the part of the Bureau and the Executive Committee. This work will be made more effective and easier for all concerned if certain modifications of procedure can be made as recommended later on in this report. First we report a series of actions and recommendations since the last IUPAC Conference.

#### I. Nominations

The Division Committee has approved the nominations of Dr. H. GRÜNEWALD of *Angewandte Chemie*, Heidelberg, as Associate Member of the Organic Nomenclature Commission (III.1) and of Mr. S. P. KLESNEY of the Dow Chemical Co., Midland, Michigan, as Titular Member and Secretary of the Commission to succeed Dr. H. S. NUTTING, who has retired. These appointments have been approved by the Bureau and the Executive Committee.

#### 2. Commissions

III.1, *Organic Nomenclature*—The report of Prof. P. E. VERKADE (Chairman) is given in Appendix A. (By an unaccountable error, the latest *IUPAC Address List* reports Dr. K. L. LOENING as Chairman of this Commission.)

This Commission is active, has accomplished a good deal, and there is a continuing need for its activity. I recommend that it be continued in its exceptional status as a Commission without expiration date.

III.3, *Joint Commission on Biochemical Nomenclature*—(This Commission is incorrectly listed in *Comptes Rendus XXIV Conference* with the number III.2. There was already a Commission III.2 at the time this Joint Commission was assigned to the Organic Chemistry Division, and hence the Joint Commission is III.3.) This Commission was assigned to the Organic Chemistry Division by the Bureau at the time of the dissolution of the Biological Chemistry Division. Its mission differs from that of III.1 in being more specialized and of great concern to the IUB Commission of Editors of Biochemical Journals, and also in its activity in the area of abbreviations, symbols, and trivial terminology. The Secretary of the Commission, Dr. W. E. COHN of the Oak Ridge National Laboratory, USA, is also Director of the NAS-NRC Office of Biochemical Nomenclature.

The interests of these Commissions do overlap, and each sends an Observer to the meetings of the other. Joint Sub-Committees of III.1 and III.3 have completed reports on cyclitols and steroids and are working on carbohydrates and carotenoids.

It is clear that it would be inefficient to try to combine these differently oriented Commissions. IUPAC's co-sponsorship of III.3 is probably a help in promoting the close collaboration of the two nomenclature bodies. I therefore recommend continuance of Commission III.3 until such time as a more favourable administrative arrangement may be found.

III.2, *Chemical Plant Taxonomy*—By a most unusual error, all mention of this Commission is omitted from *Comptes Rendus XXIV Conference* and the latest *IUPAC Address List*. The Commission was set up in 1965 and since its official creation it has held only a single meeting (Stockholm, 28th and 30th June, 1966). A second meeting is scheduled for Cortina d'Ampezzo, 2nd July, 1969.

The Commission originated in a congenial group which had been meeting informally for several years. Paradoxically, it seems to have been less active since it became a Commission than it was before. Its mission lacks the generality or urgency of the other two Commissions of Division III and the case for its continuance appears correspondingly less strong. Also, there are other bodies now carrying on some of the work for which this Commission was organized.

### 3. Sponsorship

Symposia held:—

*Valence Isomerization*, Karlsruhe, 9-12th September, 1968: Hard working, very successful, attendance 200.

*VIth Chemistry of Natural Products (Steroids and Terpenes)*, Mexico City, 21-25th April, 1969.

*IInd Pre-Symposium on Carotenoids other than Vitamin A*, Las Cruces, New Mexico, 6-9th May, 1969.

Symposia approved:—

*Conformational Analysis*, Brussels, 8-12th September, 1969.

*VIIth Chemistry of Natural Products*, Riga, 22-27th June, 1970.

*IIIrd Photochemistry*, St. Moritz, 12-18th July, 1970.

*Nonbenzenoid Aromatic Compounds*, Sendai, 25-30th August, 1970.

*Cycloaddition*, Munich, 14-17th September, 1970.

Symposium recommended:—

*Vth Carbohydrate Chemistry*, Paris, 17-22nd August, 1970.

Symposia contemplated:—

*New Synthetic Methods*

*Organic Reaction Mechanisms*

#### 4. Outside Proposals for Commissions

1. *Therapeutic Chemistry*—proposed at the XXIVth Conference (Prague), where it was decided to ask Prof. P. A. PLATTNER to chair an *ad hoc* study group to report on desirability. Prof. PLATTNER gave his oral opinion on 21st October, 1968:

A problem exists in improving standards of therapeutic chemistry, which is best solved through contact and joint action with those bodies (primarily medical) already chiefly concerned with production and publication of research in the field. He cited the World Health Organization (WHO) and Food and Agriculture Organization (FAO), two UNESCO agencies, and proposed that the Secretary General undertakes to establish contact with these bodies with the purpose of having one or more qualified therapeutic chemist added to their committees which deal with standards. At the least, this would remind WHO of the availability of needed chemical advice through IUPAC.

2. *Organic Photochemistry*—At the XXIVth Conference (Prague) it was decided to ask Prof. G. S. HAMMOND to chair an *ad hoc* study group in this field. The group consists of Prof. HAMMOND, Prof. G. J. HOYTINK, and Prof. G. QUINCKERT, but as of the date of this report, no recommendation has been received from it.

#### 5. Other Activities

The Organic Chemistry Division Committee is prepared to work out recommendations on standard practices in the publication of organic research papers. A memorandum by Prof. E. A. SHILOV has raised questions about the mandatory publication of elementary analyses. This has proved to be too far-reaching a topic to be settled by mail; after several exchanges it is on the agenda for the Cortina meeting. The Committee is also rendering a service to the Programme Committee of the forthcoming XXIIIrd IUPAC Congress (1971) to be held in Boston, by consulting on a number of matters concerned with the organic chemistry programme.

#### 6. Recommendations

The ably written Statutes and By-laws of IUPAC contemplate that most of its work will be done through meetings of Commissions, whose travel expenses constitute a major claim on the IUPAC treasury. It is our experience that an active and interested Division Committee can do as much good as



a number of Sections and Commissions, and preserve a flexibility and economy in its programme which is impossible with a large collection of specialized groups having many Titular Members. Yet in the course of such activity some need for funds inevitably arises. We strongly endorse the unanimous recommendation of the Division Presidents, made at Zürich in May, 1968, that each Division Committee be given a general budget *not* restricted to the payment of travel expenses, for the carrying on of its work from one year to the next. Small financial emergencies should be capable of being handled by a Division President from a contingency fund. In most cases it remains true that organizers of symposia need only IUPAC's blessing to raise the money that they require. But the exceptional and meritorious cases require informed and decisive action.

There are several cases in which IUPAC would be better served by a careful interpretation, and in some cases relaxation, of its rules about sponsorship. Statute 9.42, which forbids any constituent body of IUPAC to solicit outside funds for its programme, should be specially interpreted not to apply to a Division Committee organizing a symposium for which the Bureau has granted sponsorship but not a subvention. The current rule requiring approval of a sponsored meeting at least two years before it takes place is very useful for outside proposals, but should be relaxed in the case of a symposium which is part of the overall plan of a Division Committee. Flexibility is especially needed if the principle is to be maintained which excludes sponsored meetings in a Congress year.

The Division President served as official representative of IUPAC at the opening of the *VIIth International Symposium on the Chemistry of Natural Products* at Mexico City, 21-25th April, 1969. The symposium was attended by 289 chemists from 22 countries; it had ten plenary lectures, five days of sessions, an opening reception and closing dinner, several concerts and entertainments, a ladies' programme, and post-symposium visits to Mexican Petroleum Institute, Syntex SA-Experimental Farm, Syntex SA, Proquina SA. It was co-sponsored by 28 organizations, most actively by the Sociedad Química de México.

It is expected that the new Division President will represent IUPAC at the Brussels *Symposium on Conformational Analysis*, 8-12th September, 1969.

## 7. Budget

Most of the items required are routine. The reasons have been explained above why the responsibility and activity of the Division Committee requires an annual rather than a biennial meeting, and also why a divisional programme-and-contingency fund is needed (larger in the non-Congress year 1970 than in 1969).

For the Riga *VIIth International Symposium on the Chemistry of Natural Products* the Academy of Sciences of USSR plans to provide all the expenses of the invited speakers from Moscow to Riga and return, and for a two-week stay in the Soviet Union. The requested amount is to cover the expenses of these guests from their homes to Moscow and return.

The estimate for 1970 assumes that one new Commission may be set up, and an existing one terminated.

1969

Division Committee (Cortina d'Ampezzo), 10 Titular	\$
Members .. .. .	3,960
Commission III.1 (Oberursel), 8 Titular Members ..	2,284

Commission III.2 (Cortina d'Ampezzo), 8 Titular Members (3 duplications) .. .. .	2,837
Commission III.3 (New England), 5 Titular Members .. .. .	2,522
Administrative expenses .. .. .	100
Division programme-and-contingency fund .. .. .	2,000
VIth Natural Products Symposium, Mexico City, April .. .. .	4,000
<hr/> Total .. .. .	<hr/> 17,703

#### 1970 (Estimate)

VIIth Natural Products Symposium, Riga, June .. .. .	7,500
Photochemistry Symposium, St. Moritz, July .. .. .	2,000
Cycloaddition Symposium, Munich, September .. .. .	2,000
Division Committee .. .. .	3,960
Commission III.1 .. .. .	2,284
Commission III.3 .. .. .	2,522
Possible new Commission .. .. .	2,500
Administrative expenses .. .. .	100
Division programme-and-contingency fund .. .. .	3,000
<hr/> Total .. .. .	<hr/> 25,766

P. D. BARTLETT  
President, Organic Chemistry Division

## Appendix A: Commission III.1

### *General Organic Chemical Nomenclature*

Since about 1949 the Commission has been engaged in the preparation of a set of rules for the nomenclature of the whole of organic chemistry. It was the first time that this very extensive, difficult and time-consuming work was undertaken; the predecessors of IUPAC Nomenclature, *Geneva Nomenclature* (1892) and *Liège Nomenclature* (1930) dealt practically only with the nomenclature of cyclic compounds.

This work will, when finished, consist of five sections, as detailed below:

*Section A: Hydrocarbons* and *Section B: Fundamental Heterocyclic Systems*, were published in their 'definitive' form in 1958—they are known as the IUPAC 1957 Rules—and have been reprinted in 1966.

*Section C: Characteristic Groups containing Carbon, Hydrogen, Oxygen, Nitrogen, Halogen, Sulfur, Selenium, and/or Tellurium*—known as the IUPAC 1965 Rules—was published in its 'definitive' form in 1966.

*Section D* is in course of preparation, where necessary in cooperation with the Commission on Nomenclature of Inorganic Chemistry (II.2). It will deal with coordination compounds, organometallic compounds, chains and rings containing heteroatoms, organosilicon compounds, organic derivations

of phosphorus, arsenic, antimony and bismuth, and organoboron compounds. A few parts of this Section have already been published in tentative form in the *IUPAC Information Bulletin*. It may be expected that the whole Section will be available for publication in a tentative form within the next year or so.

*Section E: Fundamental Stereochemistry*, is ready. It is now being prepared for printing and it is hoped that it will appear in tentative form in the course of 1969.

### *Nomenclature for Special Fields*

Work on the nomenclature of the following groups of natural products and related compounds is in progress in cooperation with the *IUPAC-IUB Commission on Biochemical Nomenclature* (III.3).

*Cyclitols*. A tentative document on this matter has been published in *IUPAC Information Bulletin* No. 32 (August 1968) and has appeared also in biochemical journals.

*Steroids*. A new set of rules (tentative) for the nomenclature in this field—an extension of that published in 1958—has been published in *IUPAC Information Bulletin* No. 33 (December 1968) and in biochemical journals.

*Carbohydrates*. A set of rules for the nomenclature in this field has been prepared and is now being brought into good form for publication on a tentative basis.

*Carotenoids*. It is hoped that work on the nomenclature of *porphyrins and chlorophylls* will start soon.

The above report includes already a lot of future work. Moreover, the Commission has started work on the revision (but only where strictly necessary) and extension of the material contained in *Sections A, B, and C* of the *IUPAC Nomenclature of Organic Chemistry* and also a study on the possibility of the creation of a new and more systematic nomenclature of organic chemistry, of course not forgetting the evident fact that a fundamental difference between new and existing nomenclature seems hardly possible. In this connection it is worthwhile to mention that a new method for naming polycyclic systems has already been worked out.

As you know, the Commission meets annually for about a week. In between these meetings much work is done by correspondence. The next meeting will take place in Germany at the end of May, 1969, thanks to the fact that Dr. H. GRÜNEWALD has joined the Commission as an Associate Member.



## IV. MACROMOLECULAR DIVISION

### Report of President

(Item 14, Council Meetings, 5th and 7th July 1969)

The formation of the Division was determined by the XXIVth IUPAC Conference in Prague 1967. At the first meeting of the Division Committee held in Brussels in November 1967 the Officers of the Division were elected and the by-laws and terms of reference were adopted. Another Division Committee meeting was held in Frankfurt in March 1968 and an informal session during the Toronto Macromolecular Symposium in September 1969.

The Division has continued and extended the activities of the former Commission on Macromolecules and of the Polymer and Plastics Section. Its object was to develop these activities without forming a number of permanent Commissions. The only Commission that has been formed and approved by the Bureau deals with nomenclature problems (IV.1). All other work is done by Working Groups, *ad hoc* Committees, and individual experts.

#### 1. Nomenclature Commission

This was formed under the chairmanship of Dr. K. L. LOENING. Its efforts should be considered as a continuation of the Committee on Nomenclature of the former IUPAC Commission on Macromolecules. The first meeting of nomenclature experts convened by the Division Committee was held in Toronto on 1-2nd September, 1968. A discussion of basic principles of polymer nomenclature resulted in the first draft of a new set of definitions based on both structure and source of polymers. These definitions were further refined during the session of the Commission in Oberursel, 3-8th June, 1969. The current programme of the Commission includes revision and extension of macromolecular nomenclature with special respect to stereochemistry and to biopolymers. Contact with the IUPAC Organic Nomenclature Commission is adequately covered by a common membership of two people. Contacts will be established with the Inorganic Nomenclature Commission and with the Joint IUB-IUPAC Commission on Biochemical Nomenclature. Connections with coding and machine language, which far exceed the macromolecular field, will be treated in the Macromolecular Division only after general decisions have been taken on this subject by the IUPAC Conference in Cortina.

#### 2. Working Groups on Properties and Structure of Polymers

In continuation of the activities of the precursor bodies of the Macromolecular Division a concerted study of well-defined samples of selected polymers was performed in two parallel and closely coordinated directions.

The Working Group on *The Relationship of Performance Characteristics to Basic Parameters of Polymers*, under the Chairmanship of Dr. J. W. BARRETT, continues the ambitious programme previously laid down in the former Polymer and Plastics Section of the Applied Chemistry Division. The collaborative technical programmes of this Working Group have been continued and extended. An important requirement of this Working Group is to publish

summaries of the results of all the collaborative projects. The first paper (T. T. JONES, Monsanto), *A Collaborative Study of Polystyrene using Torsion Pendulum and Impact Methods*, was delivered in Prague in 1965 but only just published in *Journal of Polymer Science*, Part C, No. 16, 3845 (1968). Quicker publication is now anticipated by the agreement to publish all further work in *Pure and Applied Chemistry*. The first part of the PVC study is expected to appear in the IUPAC journal in mid-1969 as a paper by A. GONZE, Solvay, entitled *A Collaborative Study of the Dynamic, Mechanical and Impact Properties of Polyvinylchloride*, and later in the year the earlier rheological studies will become available in a paper by J. L. S. WALES, T.N.O., entitled *A Collaborative Investigation into the Rheology of some Polystyrene and Polyethylene Melts*.

The Working Group on *Molecular Characterization of Commercial Polymers* was organized by its Chairman, Prof. H. BENOIT, in order to supply the first Working Group with more reliable information on average molecular weight, polydispersity, long and short chain branching, and stereoregularity. Using GPC, NMR, and many other improved techniques, over 50 different laboratories have established experimental work on common samples of polystyrene, polyvinylchloride, and polyethylene.

### 3. Education in Macromolecular Science

It was felt that there is no sound relationship between the importance and industrial significance of macromolecular science and its teaching in academic institutions. In the first session of the Division Committee in 1967, Prof. G. SMETS was asked to collect information concerning this problem and to draw up a document which could be helpful for promoting education in macromolecular fields. The preliminary report on *Teaching and Research in High Polymer Science* will be presented at the XXVth IUPAC Conference in Cortina.

### 4. Symposia and Other Scientific Meetings

The series of annual symposia was continued in the traditional way. The symposium in Brussels (1967) was followed by that in Toronto (1968) and the schedule of future symposia has been established: Budapest (1969), Leiden (1970), Boston (1971). Besides these regular symposia the Division has stimulated the organization of specialized international meetings covering very narrow subjects. The Prague Microsymposia on Macromolecules represent this kind of meeting.

O. WICHTERLE  
President, Macromolecular Division

## V. ANALYTICAL CHEMISTRY DIVISION

### Report of President

(Item 14, Council Meetings, 5th and 7th July 1969)

Since the XXIVth Conference of IUPAC, held in Prague in 1967, seven reports have been submitted to the Scientific Editor for publication in *Pure and Applied Chemistry*. Seven additional reports are in the final stages of processing by the Division.

The Division was represented at a meeting of a group from IUPAC, ILO, FAO, and IAEA to discuss the influence of analytical chemistry on economic and social development and the possibilities of setting up an International Laboratory for Analytical Chemistry. The Division was also represented by the Division President at a Working Committee Meeting which was held in Jamaica, under the auspices of the International Union for the Control of Cancer together with the International Agency for Cancer Research, to consider analytical and other problems associated with chemical carcinogens. A joint meeting of the Officers of Commissions I.3 and V.5 has been held and Commissions V.3 and V.7 have met.

*Commission V.1* has been reorganized to deal with the programme, on behalf of the CE, on the production of standard methods of analysis for the control of the purity of food additives. The methods for the 1968/9 contract have been put into a standard format and assessed by the Commission Members.

*Commission V.2*, dealing with Microchemical Techniques and Trace Analysis, is studying five aspects of organic elemental analysis which are of special interest in microanalysis. These projects involve a considerable effort in organizing experimental work and in interpretation of data. Working parties have also been set up to study mass absorption coefficients for electron beam microanalysis and the purification of reagents used in micro and trace analysis.

*The Nomenclature Commission, V.3*, is finalizing its report on liquid-liquid distribution and is progressing with its work on the regularization of terminology associated with automatic analysis, contamination phenomena in analytical precipitation and, in collaboration with Commission V.2, scales of working. Nomenclature connected with ion exchange and chromatography is being studied and an attempt is being made to produce terms that are common to these two types of separation process and to gas chromatography, for which IUPAC recommendations have already been made. The Commission is also compiling a list of trivial names of reagents, on behalf of the Inter-Divisional Committee on Nomenclature and Symbols, and is studying the need for further primary standards. Working groups have been set up to consider the usage of the terms molarity, normality, and formality, and to examine the necessity for stipulation of essential data in reports of proposed new methods of analysis.

*The Commission on Spectrochemical and Other Optical Procedures for Analyses, V.4*, has revised its report on nomenclature, symbols, and units in spectrochemical analysis, dealing with atomic emission spectroscopy, and the report is now ready for tentative publication. The Commission is currently



working on a second report for the terminology and symbols associated with flame atomic absorption and fluorescence, X-ray spectroscopy, excitation sources, and determination of detection limits.

*Commission V.5 on Electroanalytical Chemistry* has a continuing project on the purity and purification of solvents and a further report is expected early next year. Tables of dissociation constants of acids in certain non-aqueous solvents are being compiled and a start has been made on a revision of tables of oxidation-reduction potentials. Studies on the purification, and determination of purity, of reagents used in polarography and stripping methods have been started. Work on the compilation of inorganic half-wave potentials is under way as is another programme of collecting and evaluating data on voltammetry and related systems, excluding inorganic polarography.

*Commission V.6 on Equilibrium Data* has revised tables of stability constants and the new compilation should soon be available. Work on distribution and heterogeneous equilibrium constants is proceeding; chelate extraction systems and various solvent systems are being studied. Critical surveys of stability constants of selected ligands and metal ions are being prepared, some of which are now being circulated within the Commission. A grant of \$4,000 has been provided by the US National Bureau of Standards to help in the compilation of distribution equilibrium standards. The support is for two years beginning June 1968.

*Commission V.7 on Analytical Radiochemistry and Nuclear Materials* is soon issuing drafts of reports on the purity of labelled preparations, a glossary of terms used in radiochemistry, and an intercomparison of analytical methods for determination of uranium in low grade ores. Work is proceeding on publicity for radiochemical methods, reference materials for activation analysis, analysis of nuclear materials, and source materials for radiochemistry.

P. W. WEST  
President, Analytical Chemistry Division

## VI. APPLIED CHEMISTRY DIVISION

### Report of President

(Item 14, Council Meetings, 5th and 7th July 1969)

This report summarizes the activities of this Division during the period between the XXIVth Conference (Prague, August 1967) and April 1969.

The Division Committee met in Montreal on 1st and 2nd October, 1968. The work of each of our eight Sections and their Commissions and Sub-Commissions was reviewed and evaluated. Various problems in connection with publications, organization of symposia, and membership were reviewed. Particular attention was paid to liaison with industry, and how best the Applied Chemistry Division could serve industry. Various topics for world-wide symposia in fields of industrial or applied chemistry were discussed.

The following is a summary of activities of each of the Sections of the Applied Chemistry Division.

#### VI.1. Food Section

This Section, under the Chairmanship of Dr. A. C. FRAZER, operates through its two Commissions.

##### VI.1.1. *Trace Substances Commission*

This Commission, under the Chairmanship of Dr. H. FISCHBACH, has operated through two Sub-Commissions.

##### VI.1.1.1. *Sub-Commission on Mycotoxins*

This Sub-Commission, under the Chairmanship of Dr. N. R. JONES, has now completed Stage 3 of its programme on the analysis of aflatoxins. This programme has been underway for several years and has pointed out the basic difficulties involved. The further research on the stability of standards has now been completed and an international study is being organized on the stability of standards forwarded by air. This problem of the stability of standards must be solved to permit further progress. In the meantime, extensive collaborative work has been carried out on comparison of analytical methods for the various aflatoxins in selected foodstuffs. The methods have thus far not shown satisfactory agreement among collaborating laboratories and further work is required. Later, the Sub-Commission will broaden its field of endeavour to the analysis of various mycotoxins.

##### VI.1.1.2. *Sub-Commission on Smoke Constituents*

This Sub-Commission, under the Chairmanship of Dr. H. FISCHBACH, is engaged in the study of analytical methods for the determination of benzo(a) pyrene in smoked foods at part per billion levels. Further collaborative studies are proceeding in the comparative levels of accuracy of the Howard Method, adopted as official by the AOAC in 1968, and other procedures. The aim is to extend the sensitivity of the subject methods to 2  $\mu\text{g/kg}$  and to undertake study of the multi-detection method for polycyclic aromatic hydrocarbons in smoked foods. Considerable progress has been made on shortening

and improving the published Howard procedure for multi-detection of the hydrocarbons. Eventually, the Sub-Committee proposes to expand its activities to encompass extension of the established methods to analysis of smoke condensates and the development of methods for other deleterious contaminants in smoked foods, including trace elements. Specifically, there is concern about the possible presence of the highly potent carcinogens, the nitrosamines, in smoked products. Methods of adequate sensitivity ( $10\text{ }\mu\text{g/kg}$  or less) are now not available for the analysis of these substances.

#### **VI.1.2. Food Additives and Contaminants Commission**

This Commission, under the Chairmanship of Dr. J. H. BUSHILL, has continued its studies on the methods of determination of various food additives in food. Consideration is being given to a number of solvents used in food technology, their specifications and methods of analysis. These include n-hexane, ethylene dichloride, trichlorethylene, petroleum ether, acetone, propan-2-ol, ethanol, and carbon disulphide. Additional information will be collected on other solvents. Assistance has been provided to the Coordinating Committee under Prof. R. TRUHAUT carrying out work for the CE.

#### **VI.2. Fermentation Industries Section**

This Section, under the Chairmanship of Prof. H. SUOMALAINEN, has continued its activities in various phases of interest to the fermentation industries. Publication was made in 1968 of its studies in uniform methods of alcohol determination and in international standards for expressing the alcohol content of beverages and distilled potable spirits. Work has continued on a statistical survey of the world's fermentation industries, based on operating data for 1967. The first part of a study on the fermentation power of active dry baker's yeast to establish definitions and standards of performance, has been succeeded by a collaborative study in 23 laboratories around the world of the fermentation power of baker's yeast. The objective is to define procedures which give a reliable measure of quality. The results of this study will be discussed at the XXVth Conference. The Section sponsored the *IIIrd International Fermentation Symposium* in USA in 1968, and held a Section meeting on that occasion. Planned future activities of this Section include the following: a study of the problems in water pollution, a study of the foods produced by fermentation, extension of the standard for fodder yeasts to include yeasts from hydrocarbons, and the creation of a list of terms and symbols utilized in the fermentation industry.

#### **VI.3. Oils and Fats Section**

This Section, under the Chairmanship of Prof. H. A. BOEKENOOGEN, met on 2nd and 3rd October, 1968, in Vienna. In the studies on the determination of mixtures of mono-, di- and triglycerides by column chromatography, results were not entirely clear cut and the collaborative tests are being repeated, with emphasis on details of procedure. The photometric method of determination of minor quantities of glycerol in soaps has been adopted by the Section following a discussion of the results obtained in studies, and will be inserted in the Standard Methods. A potentiometric determination of the Acid Value and Saponification Value has been adopted, and will be of particular value for dark coloured oils. Consideration was given to



examination of fats by differential thermal analysis, but the conclusion was reached that such a method is not yet ready for standardization. The lengthy studies in the identification of sterols in oils and fats by gas chromatography have been completed, and a detailed standard method has been adopted for insertion in the Standard Methods. Consideration has been given to standardization of a titrimetric method for the determination of soap in soaps. Further discussions have been held on methods of determination for alaidic acid and trans-acids. Consideration has been given to the determination of chlorinated pesticides in edible oils and fats, and the detection of ruminant fat in pork fat. The Section proposes also to include in its activities the standardization of the gas chromatographic separation of fatty acid methyl esters and the preparation of these methyl esters from oils and fatty acids.

#### **VI.4. Toxicology and Industrial Hygiene Section**

This Section, under the Chairmanship of Prof. R. TRUHAUT, has continued its studies on the methods of analysis for toxic materials in the environment and in biological fluids such as urine and blood of exposed subjects, as well as the metabolites of such toxic materials.

Various methods previously adopted have now been put into form for publication. In addition, the following have been studied: the analysis in air of antimony, ozone, iron oxide dust, sulphuric acid aerosols, mercaptans, lead dust by polarographic means, hydrofluoric acid, and methyl bromide. There has also been studied carbon monoxide and benzene in blood, and phenols and lead in urine. Attention has also been paid to cholinesterase activity. A project was begun for the control of methods using indicator tubes for the control of the industrial environment.

The working group attached to this Section on the quantitative determination of cancerogenic chemicals in air has been engaged in the study of methods for aromatic polycyclic compounds, benzo(a)pyrene and nitrosamines in air, as well as elements potentially cancerogenic such as beryllium and selenium. Data on the absorption and fluorescence spectra of aromatic polycyclic hydrocarbons have been circulated.

A start has been made in the determination of various constituents of air pollution, including sulphur dioxide, carbon monoxide, and oxides of nitrogen.

Close liaison in these studies has been maintained with various world bodies, including WHO, ILO, the International Union Against Cancer, and the International Permanent Commission for Industrial Medicine.

#### **VI.5. Pesticides Section**

This Section, under the Chairmanship of Dr. H. HURTIG, together with its two Commissions met in Sittingbourne, England, on 7-9th October, 1968. The Section has continued its work in conjunction with world bodies as follows.

FAO/WHO—The programmes of the FAO/WHO Joint Meetings of Experts on Pesticide Residues and the FAO/WHO World Food Standards Programme (Codex Committee on Pesticide Residues) have in their meetings since 1966 defined problem areas in the chemistry of pesticide residues in which they consider information inadequate. An extensive compilation of information required concerning residues of over 25 pesticides was received by this Section from FAO. These have been assigned to the appropriate

Commission, depending upon whether the problem concerned a method for analysis of the residue and/or metabolites, or the elucidation of the metabolism and chemical nature of the residue, either in a raw agricultural product or in food as consumed. The progress on these problems is dealt with in very brief summary form by reports of the two Commissions. The Section was informed by the representatives of FAO and WHO that in future years, it can be expected that new problems will be passed to IUPAC: in 1969 those concerning 16 pesticides (mostly organophosphorus and carbamate insecticides), in 1970 some 12-14 fungicides, and in 1971 approximately 15 herbicides.

FAO/IAEA—This UN agency requested assistance of Titular Members of this Section in preparing background material for a special panel meeting sponsored by FAO/IAEA on the use of radio-isotopes in determining the fate of pesticide residues in raw agricultural products, in processing and in animal metabolism studies. Titular Members and others attending agreed to act in individual personal capacities, because the FAO/IAEA panel meeting was to be held in Vienna in December 1968 (not allowing sufficient time for authorization to be obtained from the Executive Committee for this Section of IUPAC to act in an official capacity). FAO/IAEA expressed its interest in collaborating actively in the work of the two Commissions.

OECD—Following a discussion of the plans under development by OECD for a special study group of member countries on environmental contamination by pesticides, it was agreed that the OECD programme was not yet at the stage for this Section of IUPAC to become involved in the problem upon which OECD anticipates need for assistance from IUPAC, *i.e.*, analytical methods for pesticide residues in animal food chains. OECD will continue to keep in touch with this Section of IUPAC on these matters.

Symposia are planned at Bonn in September 1970 on the *Chemistry of Pesticides under Metabolic and Environmental Conditions*, and in Tel Aviv in February 1971 on the *Chemical Nature of Terminal Pesticide Residues*.

#### VI.5.1. *Commission on Terminal Pesticide Residues*

This Commission, under the Chairmanship of Dr. H. HURTIG, has continued its studies requested by FAO/WHO on the nature and amount of metabolites, degradation products or residues of parent compounds of metabolites. The solution of these problems will be passed by FAO/WHO to the FAO/WHO World Food Standards Programme (Codex Alimentarius).

The following substances have been studied and their status reviewed: lindane, various cyclodienes, carbamates, organophosphorus compounds, dithiocarbamates, various organic fumigants, and methylenedioxyphenyl synergists.

This work involves not only studies on the constitution of the metabolites, but also the rate of transformation in various substrates.

#### VI.5.2. *Commission on Pesticide Residue Analysis*

This Commission, under the Chairmanship of Dr. R. A. E. GALLEY, has continued its studies of the problems assigned by FAO/WHO to be used ultimately by the FAO/WHO Codex Alimentarius Commission.

The Commission has been active particularly in studies of methods of analysis in four areas, *viz.* organochlorine compounds, fumigant residues,

organomercury residues, and organophosphorus residues. These have involved a close scrutiny of the evaluation of results obtained by highly sophisticated techniques both in multi-detection systems and in specific analyses. The quantities involved are extremely small and analysts must be specially trained in this field. The wide variety of materials show a varied response in sensitivity to the various techniques available.

#### **VI.6. Organic Coatings Section**

This Section, under the Chairmanship of Mr. P. H. FINK-JENSEN, met at Stuttgart on 30th September and 1st October, 1968, and in part also at Brussels in May 1968. A working group on information retrieval also met at Rotterdam on 26th February, 1969.

Methods of analysis for alkyd resins have been further studied, including acid, hydroxyl and saponification values, determination of phthalic anhydride and fatty acid components, and identification of type of alkyd resin. A collaborative study has been made of the gas chromatographic determination of carboxylic acids and polyols in alkyd resins. Progress has been made towards the publication of a booklet on adhesion, and a report is being prepared on the rheological properties of liquid paints. The subject of supplementary training for chemists engaged in the organic coatings industry has been studied, as well as the problems involved in information retrieval relevant to this industry.

#### **VI.7. Pulp, Paper, and Board Section**

This Section, under the Chairmanship of Dr. K. WARD, was active in arranging two international symposia, one held at Helsinki on the subject of *Recovery of Pulp Chemicals* on 13-17th May, 1968, and the other arranged for Prague on the subject of *Chemical and Physicochemical Aspects of Paper Making*, on 10-13th September, 1968. Unfortunately, the latter, owing to circumstances beyond the control of the Section, had to be cancelled.

The Section, which is not meeting at this Conference, has been active by correspondence developing a programme of future activities.

#### **VI.8. Water, Sewage, and Industrial Wastes Section**

This Section, under the Chairmanship of Dr. S. FREYSCHUSS, was reconstituted at the Prague Conference, and has been very active in the interim. Meetings have been held at Amsterdam on 18th March, 1968, at Frankfurt on 25th September, 1968, and at Brussels on 24th February, 1969.

A general programme on industrial wastes has been developed dealing with (a) sampling and measurement of flow, (b) measures against water pollution within the industrial processes, and (c) external treatment of the wastes. Each member of the Section is responsible for a specific portion of this programme. A report has been issued entitled *A Guide to Flow Measurement and Sampling with Special Reference to Pulp and Paper Mill Waste Water Systems*. A symposium is being planned for late 1970, which will deal with the various segments of industrial wastes problems. Collaboration is being planned with other Sections of the Applied Chemistry Division in industrial wastes from the various processes. The Section is also taking part in the work of COWAR, a Committee of ICSU.

W. GALLAY  
President, Applied Chemistry Division



# CLINICAL CHEMISTRY SECTION

## Report of Chairman

(Item 14, Council Meetings, 5th and 7th July 1969)

The last meeting of the Section was held in Prague on 30th and 31st August, 1967. At that meeting it became an independent Section attached to the Bureau. This was a great advance for clinical chemistry and will have great benefit for this discipline.

The next meeting of the Section will be held in September at Geneva just prior to the *International Congress of Clinical Chemistry* (8-13th September, 1969). It is fully expected that all Titular Members and many National Representatives will attend. Many will stay for the Congress which is, of course, a very important event for clinical chemists.

The functioning or working bodies of the Section are its three Commissions. These were created at the meeting in Prague and have been making good progress in their respective fields. The Commissions will meet just before the General Meeting of the Section in Geneva. Formal reports of their activities during the past two years will be presented at this General Meeting. Some details are, however, given below.

### Commission on Quantities and Units

Three meetings of the Commission were planned for in Prague. However, the Members were unable to meet together for the first of these (Copenhagen, November 1967). The first actual meeting was therefore held in Washington, DC, on 24th and 25th August, 1968. The discussions centered chiefly around the Recommendations 1966 of the IUPAC Commission (now Section) on Clinical Chemistry and the International Federation of Clinical Chemistry, as outlined in the 1966 publication *Quantities and Units in Clinical Chemistry* by R. DYBKAER and K. JØRGENSEN. Copies of this book had been sent to all National Societies of Clinical Chemistry, and considerable interest had been shown in the Recommendations by several countries, *e.g.*, Germany, UK, USA, and the Scandinavian countries. A five-page notice concerning them had been sent to about 80 editorial boards of pertinent journals and all but 9 had accepted the manuscript for publication. Members of the Commission had been asked to form part of an Expert Panel on Quantities and Units being established by the IFCC Committee on Standards. A draft of a shortened version of the Recommendations 1966 had been prepared: this was discussed in detail and several recommendations for changes and additions were made. The possibility of having translations made into other languages was discussed—this would require outside funds. It was decided to prepare a glossary of quantity names, and suggestions were made concerning other quantities to be included in the Recommendations, *e.g.*, ionic strength, osmolality, spectrophotometric units. Other related matters were discussed.

The next meeting was scheduled for June 1969 in Strasbourg; however, Dr. DYBKAER had proposed that this be held instead in Geneva in September so that the Members would be able to attend the General Meeting of the Section and the Congress as part of the same trip.

### Commission on Teaching

Meetings were held at Newcastle upon Tyne, 26th and 27th March, 1968, and at Washington, DC, 19th and 20th August, 1968. The second meeting had originally been scheduled for Paris in August 1968. SIR RONALD

NYHOLM, then the Chairman of the IUPAC Committee on Teaching of Chemistry, was called upon to provide counsel for the related programme in clinical chemistry. Prof. LATNER, a Member of our Commission, prepared a report on the teaching programme of the British Association of Clinical Biochemists. Plans were made for the preparation of a monograph on the subject of *Education and Training in Clinical Chemistry*. This will consist of an international review of the status of clinical chemistry in all countries for which information is available from the viewpoint of historical development, the present organizational status, legal development and present status, available educational programmes, and projected needs for the future. The present goal is to produce a draft monograph by September 1969. At the meeting of the Commission in Geneva, reports from various countries will be presented and the draft of the monograph will be reviewed. Consideration will be given to publication of the monograph and to publicity and distribution arrangements.

There is a close liaison between this Commission on Teaching and the similar Committee of the IFCC.

### **Commission on Automation**

The first meeting of the Commission was held in Geneva on 4th and 5th November, 1968. Previously, Prof. T. P. WHITEHEAD (UK), Dr. E. COTLOVE (USA), and Dr. K. JØRGENSEN (Denmark) had accepted invitations to serve on this Commission in addition to Dr. SANZ and Dr. J. DE WAEL (Titular Members). The Commission was established because of the importance which automation is assuming in clinical laboratories, both private and public (hospitals). Governments with social security programmes are very interested in the application of automation to population sickness surveys and screening programmes. In order for an orderly development to occur, terms must be defined and performance standards established for automatic devices. The Commission will make recommendations regarding semi-automatic as well as fully automatic systems. Methodology is also being considered.

### **Section of Clinical Chemistry**

There are a number of countries which have National Adhering Organizations of IUPAC, but which have no representation in the Section of Clinical Chemistry. Ireland, Israel, Italy, Mexico, and New Zealand can be given as examples. The Section is very interested in a broader representation among the countries of the world, and efforts will be made to contact prominent clinical chemists and the IUPAC Adhering Organizations in countries not already represented.

Dr. SANZ has received letters from Ecuador, Argentina, and Austria expressing interest in the activities of the Section. He also attended the *Ist Latin American Congress of Clinical Biochemistry* held in Mar del Plata, Argentina, in December 1968.

In summary, it can be said that the Section of Clinical Chemistry is functioning well and is carrying out several important projects which will have a pronounced effect on future developments in clinical chemistry. It is to be expected that even greater progress will be made in the near future since better channels of communication are being developed between its Officers, Titular Members, National Representatives, Commission Chairmen, and the IUPAC Secretariat. The newer Members of the Section and of the Commissions have gained valuable experience in the working and functions of IUPAC in the past two years.

A close liaison is being maintained with the International Federation of Clinical Chemistry. This is fostered by having quite a number of common Members in the two organizations as well as on Commissions and Committees. For example, Dr. SANZ and Dr. TONKS are members of the Executive Council of IFCC; and Prof. M. RUBIN (Titular Member) is also President of IFCC.

M. C. SANZ  
Chairman, Section of Clinical Chemistry



## MINUTES OF XXV COUNCIL MEETING

5th and 7th July 1969

*Present:* Prof. V. N. KONDRATIEV (President, in the Chair), Members of Bureau, Delegates of National Adhering Organizations, Delegates of Associated Organizations.

All actions necessary for the holding of a valid meeting of Council had been taken with the following letters:

*re:* Candidates for elections, 4.8.1968 (266/RM/ek) and 14.12.1968 (509/RM/ek)

*re:* Official invitation to National Adhering Organizations and Bureau Members, 2.1.1969 (537/RM/ek), 28.1.1969 (475/RR/CAD/69) and 28.1.1969 (474/RR/CAD/69)

*re:* Draft agenda, 2.1.1969 (537/RM/ek)

*re:* Official invitation to Titular and Associate Members and National Representatives, 28.1.1969 (474/RR/CAD/69)

*re:* Final agenda and candidates for elections, 30.4.1969 (891/MW/PE/69) and 8.5.1969 (750/RM/LW)

*re:* Documentation available on agenda items, 24.5.1969 and 7.6.1969 (Secretariat)

### *Minute 1 Introduction*

In his opening remarks Prof. KONDRATIEV first paid tribute to the colleagues deceased since the last Conference: E. H. BUCHNER, B. DREWS, A. C. FRAZER, O. HAHN, W. V. LEE, J. MOCKEL, J. P. WIBAUT, G. WOLFF.

The President thanked the host country, particularly Prof. G. SARTORI and his colleagues in the Italian National Committee for Chemistry and National Research Council, for all its efforts to ensure the success of the XXVth Conference. He noted that the 1st IUPAC Conference was held in Rome during 1920.

### *Minute 2 Finalization of Agenda*

At the suggestion of Prof. KONDRATIEV it was agreed to reverse the order of discussion of Items 10 and 11 from the circulated Agenda. Dr. D. C. MARTIN (UK), Dr. G. BEHRENS (Germany), and Mr. J. GIVAUDON (France) were elected as tellers for the duration of the meeting.

### *Minute 3 Minutes of XXIVth Conference Council Meeting*

The minutes of the previous Council Meeting, as circulated to the National Adhering Organizations and as printed on pages 103-112 of *Comptes Rendus XXIVth Conference*, were unanimously approved. It was noted that subsequent to the Council Meeting, the Bureau had approved a further recommendation that the Section of Clinical Chemistry be attached to the Bureau rather than the Analytical Chemistry Division.

No reply had been received by the Secretary General to his registered letter to the Luxembourg Adhering Organization re arrears in payment of dues. Luxembourg had, therefore, automatically ceased to be a member of IUPAC at the end of 1967.

*Minute 4 Nominations for Officers and Bureau Members*

The names of those proposed as Vice-President and Elected Members of the Bureau, together with biographical notes on each candidate, had been mailed in advance to all Adhering Organizations as prescribed by the Statutes and were also in the files of each Delegation. Council unanimously reconfirmed that there should be 12 Elected Members to the Bureau, so that 7 vacancies existed on this occasion.

*Minute 5 Time of Elections*

The President announced that the elections would be held on Monday, 7th July, at 11.00. The procedure for election of Officers is prescribed in the Statutes. The Bureau, according to its statutory powers, had decided (XXIIIrd Meeting) that the election of Elected Members to the Bureau should take the form of a written and secret ballot, the exact procedure for which had been conveyed in writing to each Adhering Organization at the start of the Council meeting.

*Minute 6 Report of President on State of the Union*

Prof. KONDRATIEV referred to his printed report which had been precirculated, emphasizing the need for IUPAC to improve its level of activity and its liaison with industry. The report was accepted unanimously without discussion.

*Minute 7 Biennial Report of Treasurer*

The biennial report of the Treasurer and the report of the auditors had been circulated before the meeting in printed form. Prof. BAILAR was happy to report an excess of income over expenditure of \$61,822.43 for 1967 and \$36,066.24 for 1968. He emphasized: the increasing income through the Company Associates Plan; appreciation of the support of the office of the Secretary General over several years by the four Swiss chemical companies; thanks to those employers who provided stenographic help and office facilities for IUPAC work; the generosity of some Adhering Organizations which had contributed towards the participation of their Titular Members in the XXIVth and XXVth Conferences; the excellent financial return from recent investments. On the expenditure side, the largest item was travel to meetings, which would increase further from the activities of new units; the Secretariat at Oxford and the office of the Secretary General in Zürich constituted new expenses. Finally, thanks were expressed to Schweizerische Bankgesellschaft for its excellent and generous service, which was to be more realistically recompensed in future.

*Resolved:*

That the Treasurer's biennial report be accepted and that the mandatory \$10,000 annual transfers to reserves be terminated, effective with the current fiscal year.

*Minute 8 Report of Finance Committee*

The Chairman, Mr. P. M. ARNOLD, indicated that the Finance Committee met annually in Zürich to review IUPAC financial matters. The minutes of the 1969 meeting were included in the

Council files. Its recommendations had already been implemented by the Executive Committee except for those drawn up at Cortina d'Ampezzo.

*Resolved:*

- (i) That Membership of the Finance Committee be increased from 5 to 6 Titular Members.
- (ii) That if IUPAC sponsorship is given to a meeting, the following are guiding principles with respect to social events:
  - a. Elaborate and expensive social events are discouraged.
  - b. To the end that attendance by young chemists may not be hindered, the cost of social events should not be included in the registration fee for the meeting.
  - c. The cost of social events should be paid by those who attend them, or
  - d. The cost should be financed from sources within the host country.
- (iii) As a condition precedent to IUPAC sponsorship, the organizers of a symposium or other meeting:
  - a. Shall inform IUPAC of the expected magnitude and of the sources of funds needed to finance the meeting, and
  - b. Shall agree that funds will be solicited only in an amount and from sources approved by the National Committee for IUPAC of the host country.

*Minute 9 Applications for Change of Category*

The Adhering Organizations of Brazil, Japan, and Romania had filed applications for transfer from Category B 1 to C, A 1 to A 2, and C to B 1, respectively. In a non-scientific vote by Delegations, Council accepted these transfers but ruled that they become operative after the close of the meeting and not be backdated.

*Minute 10 Budget Estimates for 1970 and 1971*

In submitting these estimates the Treasurer explained that many of the items in them are subject to change or removal because a precise budget cannot be compiled until all IUPAC Units have submitted their programmes in detail. Also, the cost of meetings would alter as a result of changes in membership of various units implemented at Cortina d'Ampezzo. Prof. BAILAR strongly recommended Adhering Organizations to deduct 5% of the income from Company Associates for use in further promotion of the Plan. He emphasized that the contingency fund of \$2,000 to each Division was a new idea on trial for 1969.

*Resolved:*

That, subject to the above provisos, the budget estimates for 1970 and 1971 be approved.

*Minute 11 Annual Dues for 1970 and 1971*

Mr. ARNOLD reported that the present scale of dues to be paid by Adhering Organizations, taken in conjunction with other sources of revenue, will be adequate to support IUPAC activities now foreseen for 1970 and 1971.



*Resolved:*

That the minimal annual dues of member countries for 1970 and 1971 be fixed as follows:

Category D	\$100
Category C	\$450
Category B 1	\$800
Category B 2	\$1,600
Category A 1	\$2,600
Category A 2	\$5,000
Category A 3	\$10,000
Category A 4	\$25,000

*Minute 12 Dues Structure*

The President reminded Council that at the XXIVth Conference, in order to provide IUPAC with sufficient income to support its present level of activity, the USA Delegation had proposed a revision of the annual dues structure. Subsequently, the Adhering Organizations had been asked to comment on a dues scheme in which membership categories were related to the national chemical turnover of the member countries. A memorandum from the Treasurer summarized the present thinking on the new dues scheme; a second document in the files, prepared by an *ad hoc* Committee of the Bureau, presented the scheme in the form of three principles:

- (i) Chemical turnover as the basis of a new dues structure.
- (ii) Payment of travel expenses to be accounted as part of the dues.
- (iii) Contributions from Company Associates and other organizations to be accounted as part of the dues.

Principles (ii) and (iii) will only be voted on when Adhering Organizations have had time to consider their implications.

Following a general discussion initiated by the President, in which Delegates from Netherlands, Hungary, Japan, South Africa, Ireland, Germany, Sweden, and Turkey took part, it was clear that clarification is needed of exactly which industries are considered to contribute to national chemical turnover.

*Resolved:*

That the principle of chemical turnover as the basis of a new dues structure be referred back to the Finance Committee for precise definition of the term 'chemical turnover'.

*Minute 13 Committee on Teaching of Chemistry*

The printed report of the Committee on Teaching of Chemistry was included in the Council files. In referring to the status of existing programmes, the Chairman, Prof. R. W. PARRY, requested Adhering Organizations to bring the report on *In-service Training of Chemistry Teachers* to the attention of Ministries of Education and other national organizations concerned with the supply and training of chemistry teachers. Active collaboration, under contract, had been established with UNESCO. The Committee is starting to sponsor and participate in international symposia on chemical education. New programmes being initiated include an investigation into the supply and training of

chemistry technicians. Council approved the report and unanimously endorsed the importance of the work being undertaken by the Committee.

*Minute 14 IUPAC Publications*

Sir HAROLD THOMPSON informed Council of the important points from his report as Chairman of the Editorial Advisory Board and from the report of the Scientific Editor (Prof. B. C. L. WEEDON) and of the recommendations of an *ad hoc* Committee on Publications convened by the Executive Committee, all of which had been presented to the Bureau (XXIIIrd Meeting).

With a sum of \$10,200 received by IUPAC from its publishers in 1968, the falling royalties in recent years had been amply reversed. Through the appointment of Symposium Editors it was hoped to avoid previous delays in publication of proceedings of symposia. There seemed a very good chance of completing the three volumes of *Pure and Applied Chemistry* scheduled for 1969 by about the end of the year. The rapid growth in number of symposia being sponsored by IUPAC might make it necessary to apply some selectivity in regard to those the Union decides to publish. New mechanisms are proposed for distribution of the *Information Bulletin* and *Comptes Rendus* and for publication of tentative and final nomenclature rules. Some thought would need to be given to the content and use of the *Bulletin* in view of the changed publication of tentative rules.

*Resolved:*

That, in receiving the report on publications and endorsing the new mechanisms for publication of nomenclature rules, a vote of thanks from Council be minuted to Sir HAROLD THOMPSON and Prof. WEEDON for their work for the Union.

*Minute 15 Reports of Division Presidents and Clinical Chemistry Section*

The Division Presidents referred briefly to their precirculated reports of activity since the XXIVth Conference, then informed Council of the further progress made during the XXVth Conference. It was not possible to update the Clinical Chemistry Section report because the Section was not meeting until September, but the Chairman, Dr. M. C. SANZ, anticipated that the Section would meet in future during Conference. Sir HARRY MELVILLE, President of the Physical Chemistry Division, indicated that relations between IUPAC and CITCE had been satisfactorily normalized. It is now understood that matters of electrochemical nomenclature are the concern of Commission I.3. CITCE will function as an international society of electrochemistry which organizes scientific meetings, but not publish any nomenclature proposals under its auspices. Council agreed to receive the reports and

*Resolved:*

- (i) That IUPAC strongly supports Recommendation U1 (1969) of the Comité Consultatif des Unités that the mole be recognized as an SI Base Unit, and urges the Comité

International des Poids et Mesures to present it with full support to the XIVth Conférence Générale des Poids et Mesures.

- (ii) That IUPAC recommends the Advisory Committee on Thermometry to adopt the melting point of alumina as a secondary standard for the International Practical Temperature Scale.

*Minute 16 Ratification of Decisions taken by Bureau and Executive Committee since XXIVth Conference*

All decisions taken by the two bodies were contained in the approved Minutes of the XXIst and XXIIInd Bureau and LIX-LXIVth Executive Committee meetings, which were in the hands of all Delegates. The Council

*Resolved:*

That the decisions taken by the Bureau and Executive Committee since the XXIVth Conference be ratified.

*Minute 17 Elections*

The President informed the meeting that all the necessary voting papers were in the hands of the tellers, who would distribute them to the Delegations.

*Present:*

35 Delegations with a total of 140 votes, in addition to which the voting rights of Brazil (4), which was not represented in Council, were officially delegated to Argentina.

*Officers:*

In a written and secret ballot for election of the Vice-President:

Prof. J. BÉNARD 140

Total voting 144, simple majority 73.

The meeting rose and with acclamation congratulated Prof. BÉNARD as the new Vice-President.

*Elected Members to the Bureau:*

In a written and secret ballot (see Minute 5) for 7 vacancies.

*First Ballot:*

Mr. P. M. ARNOLD	127
Prof. G. SMETS	117
Prof. H. MALISSA	104
Prof. H. SUOMALAINEN	95
Prof. S. RANGASWAMI	79
Prof. V. HEROUT	77
Prof. L. H. BRIGGS	64
Prof. M. CAIS	60
Dr. P. R. GENDRON	60
Prof. G. SCHAY	57
Dr. W. ZATTAR	52
Prof. E. A. M. DAHMEN	44
Prof. F. L. WARREN	39
Prof. TONG HYUK AHN	23

Total voting 1008, simple majority 73.



6 vacancies were declared to be filled by Mr. ARNOLD, Prof. SMETS, Prof. MALISSA, Prof. SUOMALAINEN, Prof. RANGASWAMI, and Prof. HEROUT.

*Second Ballot:*

Dr. P. R. GENDRON	40
Prof. L. H. BRIGGS	34
Prof. M. CAIS	34
Prof. G. SCHAY	18
Prof. E. A. M. DAHMEN	6
Prof. F. L. WARREN	5
Dr. W. ZATTAR	4
Prof. TONG HYUK AHN	3
Total voting 144, simple majority 73.	

*Third Ballot:*

Dr. P. R. GENDRON	65
Prof. L. H. BRIGGS	36
Prof. M. CAIS	29
Prof. G. SCHAY	8
Prof. F. L. WARREN	6
Dr. W. ZATTAR	0
Prof. E. A. M. DAHMEN	0
Total voting 144, simple majority 73.	

*Fourth Ballot:*

Dr. P. R. GENDRON	73
Prof. L. H. BRIGGS	30
Prof. M. CAIS	19
Prof. G. SCHAY	16
Prof. F. L. WARREN	6
Total voting 144, simple majority 73.	

The remaining vacancy was declared to be filled by Dr. GENDRON.

The meeting offered its congratulations to the 7 newly Elected Members to the Bureau.

The following elections of Officers made by the Divisions were approved by Council:

*Physical Chemistry Division*

President (1969-1973):	Dr. G. WADDINGTON
Vice-President (1969-1973):	Prof. J. Th. G. OVERBEEK
Secretary (1969-1973):	Dr. R. N. JONES

*Inorganic Chemistry Division*

President (1969-1973):	Prof. O. GLEMSE
Vice-President (1969-1973):	Prof. V. GUTMANN
Secretary (1967-1971):	Prof. R. COLLONGUES

*Organic Chemistry Division*

President (1969-1971):	Prof. D. H. R. BARTON
Vice-President (1969-1971):	Prof. G. OURISSON
Secretary (1969-1973):	Prof. A. KJAER

*Macromolecular Division*

President (1967-1971):	Prof. O. WICHTERLE
Vice-President (1967-1971):	Prof. H. BENOIT
Secretary (1967-1971):	Prof. G. SMETS

*Analytical Chemistry Division*

President (1969-1973):	Prof. W. KEMULA
Vice-President (1969-1971):	Prof. P. W. WEST
Secretary (1967-1971):	Mr. R. W. FENNELL

*Applied Chemistry Division*

President (1967-1971):	Dr. W. GALLAY
Vice-President (1969-1971):	Dr. R. W. CAIRNS
Secretary (1967-1971):	Dr. I. E. PUDDINGTON

*Minute 18 Adoption of Nomenclature Rules*

Following the recommendation of the relevant Division President, Council

*Resolved:*

- (i) That the Manual of Symbols and Terminology for Physico-chemical Quantities and Units (Commission I.1) be adopted for publication as final nomenclature rules.
- (ii) That the Manual of Definitions, Terminology, and Symbols in Colloid and Surface Chemistry (Commission I.6) be adopted for publication as tentative nomenclature rules.
- (iii) That a revised edition of Nomenclature of Inorganic Chemistry—1957 (Commission II.2) be adopted for publication as final nomenclature rules; and that in the case of those tentative nomenclature rules for which it had not been possible to observe the By-law that a period of 8 months be allowed for receipt of observations, the By-law be relaxed.
- (iv) That Section D of Nomenclature of Organic Chemistry (Commission III.1) be adopted, when finalized, for publication as tentative nomenclature rules.
- (v) That Sections A/B and C (Commission III.1) be reprinted as final nomenclature rules, the reprint to incorporate some corrections and a few minor revisions.
- (vi) That Nomenclature of Carbohydrates and Nomenclature of Carotenoids (Commission III.1) be adopted, when finalized, for publication as tentative nomenclature rules.
- (vii) That Definitions in Polymer Science, Nomenclature for Polymer Science, and List of Abbreviations for Polymeric Materials (Commission IV.1) be adopted, when finalized, for publication as tentative nomenclature rules.
- (viii) That Recommended Terminology for Liquid-liquid Distribution and Extraction and Recommended Terminology for Automatic Analysis (Commission V.3) be adopted for publication as final nomenclature rules.
- (ix) That Nomenclature, Symbols, Units and Their Usage in Spectrochemical Analysis (Commission V.4) be adopted for publication as tentative nomenclature rules.
- (x) That Recommendations on Ion Exchange Nomenclature (Commission V.3) be adopted for publication as tentative nomenclature rules.

*Minute 19 Bureau Proposals for New Units*

Following the recommendations of the Bureau and Division Presidents, which were in the hands of all Delegates in printed form, Council

*Resolved:*

- (i) That IUPAC, as Parent Union of the Joint Commission on Applied Radioactivity, recommends to ICSU that the Commission be terminated and the balance of \$1,713.26 be refunded to the ICSU Treasurer.
- (ii) That all existing IUPAC Sections and Commissions be allowed to continue in existence.
- (iii) That the IUPAC-IUB Liaison Committee be a Standing Committee attached to the Bureau and the IUPAC Members be:
  - Dr. R. MORF (Switzerland), Secretary General
  - Prof. W. KLYNE (UK)
- (iv) That the Joint Commission on Biochemical Nomenclature henceforth be attached to both the Organic Chemistry and Macromolecular Divisions, and the appointments of the following IUPAC Members be renewed:
  - Dr. W. E. COHN (1969-1973)
  - Prof. W. KLYNE (1969-1973)
- (v) That a Standing Committee on Publications be appointed to advise the Bureau on all matters including policy on IUPAC publications, its composition to be:
  - Sir HAROLD THOMPSON (UK), Chairman
  - Dr. L. C. CROSS (UK)
  - Dr. H. GRÜNEWALD (Germany)
  - Dr. R. L. KENYON (USA)
  - Prof. B. C. L. WEEDON, Scientific Editor (ex-officio)
  - Dr. R. MORF, Secretary General (ex-officio)
  - Dr. M. WILLIAMS, Executive Secretary (recorder)
- (vi) That an Inter-Divisional Committee on Machine Documentation, attached to the Bureau, be appointed to work on methods for standardization and codification in the machine handling of chemical information, its composition (1969-1973) to be:
  - Dr. C. SUHR (Germany), Convenor
  - Dr. J. W. BARRETT (UK)
  - Prof. J. E. DUBOIS (France)
  - Dr. J. B. VAN EYK VON VOORTHUYSEN (Netherlands)
  - Dr. R. N. JONES (Canada)
  - Dr. H. SCHENK (Switzerland)
  - Dr. F. A. TATE (USA)
  - USSR representative (to be suggested)
- (vii) That a Sub-Commission on Plasma Chemistry (I.2.1) be appointed to initiate appropriate activities from the field of plasma chemistry, its composition (all as Associate Members) to be:
  - Dr. C. W. BECKETT (USA), Chairman
  - Dr. L. DEFFET (Belgium)
  - Dr. V. V. SYTCHEV (USSR)



- (viii) That a Commission on Organic Photochemistry (III.3) be appointed to promote international agreement on nomenclature, *etc.*, within this field, its composition (1969-1973) to be:

Prof. G. S. HAMMOND (USA), Chairman  
Prof. G. QUINKERT (Germany), Secretary  
Maximum of 6 other Titular Members (to be suggested)

- (ix) That a Section on Medicinal Chemistry (III.4) be appointed to deal internationally with the scientific chemical aspects of the subject, its composition (1969-1973) to be:

Prof. E. CAMPAIGNE (USA), Chairman	}	Titular Members
Dr. L. STERNBACH (USA), Secretary		
Prof. A. ALBERT (Australia)		
Dr. A. J. ARIENS (Netherlands)		
Dr. F. L. ROSE (UK)		
Dr. P. SENSI (Italy)		
Dr. K. TAKEDA (Japan)		
Prof. V. A. YAKOVLEV (USSR)	}	Associate Member
Dr. L. G. HUMBER (Canada)		

*Minute 20 Date and Place of XXVIIth Conference and XXIVth Congress (1973)*

On behalf of Prof. H. BREDERECK, Chairman of the Deutscher Zentrallausschuss für Chemie, Prof. O. GLEMSEK invited IUPAC to hold its XXVIIth Conference and XXIVth Congress (1973) in Germany. Council

*Resolved:*

That the invitation to hold the 1973 IUPAC Conference and Congress in Germany be accepted.

*Minute 21 Any Other Business*

On behalf of the Netherlands Delegation and as Chairman of Commission I.6, Prof. J. Th. G. OVERBEEK proposed that a vote of thanks be recorded to the IUPAC Secretariat for its excellent preparation of and services rendered during the Conference. The proposal was endorsed by Council. Prof. KONDRATIEV expressed his thanks to all Delegates for their attendance and attention to IUPAC matters. Then he handed over the Presidency to Dr. REES, who thanked the outgoing President sincerely for his many contributions of great value and significance to IUPAC over the past several years. This was endorsed with acclamation by Council.

*Vote of Thanks*

The incoming President wrote official letters of thanks to the hosts.

## ADDRESS OF INCOMING PRESIDENT AT CONCLUSION OF XXV COUNCIL MEETING

IUPAC has been singularly fortunate in having had as its President for the past two years a man of such unassuming distinction and kindly wisdom as Prof. KONDRATIEV. His association with IUPAC over many years has been marked by contributions of great significance and value. This is not an appropriate occasion to enumerate these in detail, but I cannot let pass the opportunity to acknowledge the highlights.

Since joining the Executive Committee in 1961, Prof. KONDRATIEV has been particularly concerned to see that all Commissions operated effectively. This is an objective of great merit, because this sector of IUPAC's activities absorbs a major proportion of our resources. In his quiet and unobtrusive way, he has initiated activity in a number of areas and revived activity in others.

One of IUPAC's greatest problems has been to make those industries throughout the world that are dependent on chemistry more aware of IUPAC's work. Prof. KONDRATIEV has repeatedly stressed the need for more intensive effort directed to this end. He was personally largely responsible for influencing Soviet industry to become actively interested in IUPAC.

Those of us who were privileged to attend the great XXth Congress in Moscow in 1965 retain many pleasurable memories; we recall with admiration the masterly organization of this meeting under Prof. KONDRATIEV's Chairmanship and the cordial hospitality of our Russian hosts.

More recently, Prof. KONDRATIEV has presided over the transition from IUPAC's dependence on the generosity of Swiss chemical industry to the assumption of complete financial responsibility for the maintenance of its Executive Secretariat. As you might well imagine, such a change has not been without its problems. That the transition has been effected with such success is a tribute to Prof. KONDRATIEV's quiet, but firm leadership.

As incoming President, I am glad that I shall continue to have the benefit of the advice and experience of our immediate Past-President. I am sure that all members of this Council would wish me to thank Prof. KONDRATIEV for his many valued contributions to IUPAC and for the distinction with which he has graced the Presidential Office.

Mr. President, in conveying to you this Council's sincere thanks for all that you have done for IUPAC, may I wish you every success and happiness in the future.

A. L. G. REES

# COMMITTEE ON CONGRESS ORGANIZATION AND PROGRAMMES

2nd July 1969

*Present:* Dr. G. AULIN-ERDTMAN, Dr. R. MORF from IUPAC Standing Committee; Mr. P. M. ARNOLD, Prof. J. C. BAILAR, Jr., Prof. P. D. BARTLETT, Dr. B. C. McKUSICK, Prof. C. G. OVERBERGER, Dr. M. A. PAUL from XXIIIrd IUPAC Congress Organizing Committee.

1. This meeting represented the first attempt by the IUPAC Standing Committee to collect information and offer suggestions concerning a forthcoming IUPAC Congress, *viz.* the XXIIIrd Congress to be held in Boston, Massachusetts. The meeting was convened at the request of Prof. P. D. BARTLETT, Chairman of the US National Committee for IUPAC and Programme Chairman of the XXIIIrd Congress Organizing Committee, which is headed by Dr. C. H. GREENEWALT.

Dr. MORF greeted the representatives of the Congress Committee and asked Dr. AULIN-ERDTMAN to take the chair.

2. The Chairman briefly summarized the task of the Standing Committee and indicated some means by which it might help organizers of forthcoming congresses, *e.g.*

a list of desiderata as regards topics for congresses;

recommendations regarding various details in the organization of IUPAC Congresses (based on existing documents).

It is the opinion of the Standing Committee, however, that the organizers of congresses must have full freedom to consider local conditions and other special circumstances and, whenever indicated, let those conditions influence or determine the arrangements.

3. Dr. PAUL reported on the preparations for the XXIIIrd Congress, to be held from 25th-31st July, 1971, and the opinion and advice of the Standing Committee was sought on several points. The Standing Committee made the following suggestions and recommendations:

(a) It is important that information regarding the scientific content of congresses be made available early, so that possible participants have ample time to plan for their participation. Circular 1 of the Boston Congress will be ready for distribution two years ahead of the actual meeting.

(b) Distribution of abstracts of contributed papers to registrants in advance of the congress can be useful in stimulating significant discussion at the meeting and may also facilitate decision on participation on the part of chemists from distant places.

(c) To provide for the possibility of admitting last-minute papers on recent discoveries some open time might be reserved in the programme.

(d) Strict adherence to time-schedule should be maintained. This can be brought about by firm instructions to chairmen and secretaries of sessions.

(e) Several means may be used for improving the effectiveness of the practical arrangements at congresses, *e.g.*

control over the number and legibility of slides presented with a given paper;

provision of a sufficient number of aisles between seats to facilitate entry and exit by the audience;

clear direction signs within the area of the congress for locating the various sessions;

easily legible name badges.



(f) Travel advice and assistance should be provided, particularly for congress participants unfamiliar with travelling in the host country. Such advice and assistance could include a reception desk at the international airport where travellers could receive advice on local transportation. Ample direction signs should be provided in the area surrounding the congress headquarters. A hospitality centre staffed by attendants speaking several languages is planned at the headquarters of the Boston Congress.

(g) It is considered desirable at an international congress to have an opening ceremony. Aside from ceremonial greetings a lecture with substantial scientific content, yet understandable for accompanying members, should be given during the opening ceremony. The US Organizing Committee intends to invite two principal speakers for about 20 minutes each. One of these speakers will be the President of the National Academy of Sciences, Dr. PHILIP HANDLER; the other will be a well-known industrial chemist. These speakers will present substantive views on science policy and international cooperation.

The US Organizing Committee feels that in order to allow adequate time for presentation and discussion of papers within the time available for the Boston Congress it may be necessary to restrict the number of papers accepted for presentation. Thought is being given to the possibility of arranging discussions of submitted papers without preceding oral presentation. The Standing Committee expressed the view that encouragement should be given to participation in congresses by many persons who do not present papers themselves. It was hoped that agencies supporting travel to international meetings might be willing to allow for this valuable form of participation.

Dr. PAUL presented galley-proofs of Circular 1. This circular is to be distributed at the time of the 1969 Congress in Sydney. Various additional channels for its distribution were discussed. The most promising of these seem to be the National Adhering Organizations of IUPAC, the mail chain of the *Information Bulletin*, the Company Associates of IUPAC, national chemical societies and chemical engineering societies, and personal contacts.

The impression of the Standing Committee was that the great care in preparation taken by the organizers of the Boston Congress should ensure a highly successful meeting.

4. Dr. PAUL briefly presented preliminary plans for hosting the XXVIth IUPAC Conference which will be held in Washington, DC on 19th-24th July 1971.

5. The participants felt that this meeting had been well worthwhile and that effective liaison had been established between the two Committees.

# COORDINATING COMMITTEE FOR ANALYTICAL METHODS

*1st and 5th July 1969*

*Present:* Prof. R. TRUHAUT (in the chair), Prof. R. BELCHER (5th July only), Dr. H. EGAN, Dr. W. GALLAY, Prof. H. MALISSA (1st July only), Dr. R. MORF, and Prof. P. W. WEST.

1. After transmission of apologies from Lord TODD, who was unable to attend, Prof. TRUHAUT referred with deep emotion to the death of Dr. ALASTAIR FRAZER, Chairman of the Food Section, and paid an appropriate tribute to his contribution to the work of the Committee. He also conveyed to Dr. MORF a special welcome, expressing the regrets of the Members of the Committee about his severe car accident at the end of April and their wishes for a prompt recovery to Mrs. MORF.

2. Prof. TRUHAUT reported on the Coordinating Committee meeting in London on 10th April 1969 and the action taken in conformity with the schedule adopted by that meeting for the preparation of the final wording of the 28 methods selected.

3. Dr. MORF indicated that after receiving the comments of the Food Section, he was obliged to have the 28 methods neatly typed for photo-offset printing. Because of his car accident it was necessary and urgent that the typing be done by a very competent typist under the supervision of a chemist who knows the technical matter. Prof. SIMON of the ETH in Zürich, recognizing the precarious situation and wishing to help Dr. MORF, was prepared to lend a special typewriter and to have the methods retyped in a uniform way by his former secretary. Dr. MORF further indicated that the Coordinating Committee, Section, and Commission involved in this task, were still entirely free to disregard out of the 28 methods all those which were not of high quality.

Prof. MALISSA objected to this action and it was resolved to wait the results of the various meetings dealing with CE affairs in Cortina, before taking any decision. Consequently, it was agreed to hold another meeting of the Coordinating Committee on 5th July after the Council Meeting.

4. Prof. TRUHAUT said that he was ready to send those present any basic documentation they might need for the achievement of the cooperative programmes between IUPAC and other international organizations engaged in analytic control of the environment, including food.

5. After an exchange of views on the minutes of the meeting of the Coordinating Committee in Eastbourne (March 1968) relating to the working procedure, the members agreed to discuss this question again at the meeting of the Coordinating Committee on 5th July.

6. (The meeting resumed on 5th July.) Dr. EGAN said that he understood from Prof. MALISSA that the Commission on Analytical Reactions and Reagents had examined the 28 methods proposed under the current IUPAC-CE contract and considered that more laboratory work was needed on methods Nos. 1, 3, and 19, that methods Nos. 2A/B, 4, 5, 6, 7, 8, 9, 10, 11, 15, 16 appeared to be acceptable subject to rewording; methods Nos. 17, 18 were rejected and methods Nos. 20, 21, 22, 23, 24, 25 were acceptable.

7. Prof. TRUHAUT asked how the current contract should now be progressed. It was suggested that the acceptable methods, together with (some of) those which were to be reworded, could be used in fulfilment of this and that CE be informed that these were available subject (in the case of the latter) to

rewording which was currently in progress: it was understood that the Commission was giving attention to this task.

8. Prof. TRUHAUT also raised the question of procedure for the next (10) methods for the contract and circulated copies of CE document 6931/VI/66-F dated 4th May 1966 from which these methods should be selected. Dr. EGAN referred to the draft minutes of the joint meeting between the Commission on Analytical Reactions and Reagents and the Food Section held in Cortina (also circulated) and said that, subject to the agreement of these minutes, the Food Section would in the ordinary way be responsible for the initial selection of methods for evaluation.

9. Prof. TRUHAUT further raised the question of procedure for progressing the evaluation and agreed to circulate to the Committee details of the earlier 'Eastbourne' scheme for postal comment within six weeks and to prepare from the comments an appropriate, revised scheme for the agreement of members.

10. Prof. TRUHAUT made it clear that the methods were required by CE for regulatory purposes.

11. Dr. MORF said that the financial position regarding the contract arrangements was satisfactory and it was agreed that where expedient, documents during the course of IUPAC evaluation could be handled by the IUPAC Secretariat at Oxford.

12. Prof. TRUHAUT referred to the earlier (47) CE methods and said that comments on these were due from the CE Scientific Commission. When these comments were available, they should be considered by the IUPAC Coordinating Committee.

13. It was agreed to recommend to the Bureau that the Chairmen of the following IUPAC Units should be coopted to the Coordinating Committee on Analytical Methods: Applied Chemistry Division and its Food, Pesticides, and Industrial Hygiene and Toxicology Sections; the Analytical Chemistry Division and its Commission on Analytical Reactions and Reagents.



# FINANCE COMMITTEE

2nd July 1969

*Present:* Mr. P. M. ARNOLD (in the chair), Dr. J. W. BARRETT, Mr. M. J. BROCARD, Dr. C. O. GABRIELSON, Prof. O. HORN, Dr. R. MORF; Prof. V. N. KONDRATIEV and Prof. J. C. BAILAR, Jr., specially invited.

## 1. Membership of Committee

The resolution of Council establishing the Finance Committee provided that it should have a membership of not more than five members. The Committee believed that it would be useful to have an additional member. Therefore, it offered the following resolution to Council:

Be it resolved that:

The membership of the Finance Committee is increased to a maximum of six members.

## 2. Company Associates

In view of the important financial contributions being made by the Company Associates, it is desirable for IUPAC to maintain their interest. The Finance Committee noted the decision of the Macromolecular Division to supply the Company Associates with summary reports of the results of collaborative work on physical properties and molecular characteristics of commercial polymers, and it recommended that other Divisions give favourable consideration to sending Company Associates copies of documents having industrial utility or importance.

## 3. Social Events

The costs of social events held in conjunction with IUPAC-sponsored meetings have been increasing. While the expenses of past social events have not been paid by IUPAC, the Finance Committee felt some concern that IUPAC funds in the future might be spent for social affairs by organizers of symposia or other meetings. Also, the inclusion of the cost of social events in the registration fees for meetings may hinder attendance by younger chemists. Therefore, the Finance Committee offered the following resolution to Council:

Be it resolved that:

If IUPAC sponsorship is given to a meeting, the following are guiding principles with respect to social events:

- (a) Elaborate and expensive social events are discouraged.
- (b) To the end that attendance by young chemists may not be hindered, the cost of social events should not be included in the registration fee for the meeting.
- (c) The cost of social events should be paid by those who attend them, or
- (d) The cost should be financed from sources within the host country.

## 4. Financing of Symposia

In some cases, organizers of symposia or other meetings had sought funds from industrial and other organizations in many countries. The Finance Committee believed that fund solicitation by others, using IUPAC sponsorship as an element of the appeal, may have an adverse effect on the financing of IUPAC itself. The Finance Committee offered the following resolution to Council:

Be it resolved that:

As a condition precedent to IUPAC sponsorship, the organizers of a symposium or other meeting

(a) shall inform IUPAC of the expected magnitude and of the sources of funds needed to finance the meeting, and

(b) shall agree that funds will be solicited only in an amount and from sources approved by the National Committee for IUPAC of the host country.

#### **5. Annual Dues for 1970 and 1971**

The Finance Committee believed that the present scale of dues to be paid by Adhering Bodies, taken in conjunction with other sources of revenue, would be adequate to support IUPAC activities now foreseen for 1970 and 1971. The Committee therefore recommended that the scale of dues continue at the present rates until the next Council meeting.

#### **6. Revision of Dues Structure**

The Committee discussed the revision of the dues structure appearing as Item 10 of the agenda for the Council meeting of 5th and 7th July, 1969. The Finance Committee reaffirmed its recommendation that such a revision in principle be adopted by the Council.

# INTER-DIVISIONAL COMMITTEE ON NOMENCLATURE AND SYMBOLS

4th July 1969

*Present:* Prof. K. A. JENSEN (in the chair), Prof. R. BELCHER, Prof. O. HOFFMANN-OSTENHOF, Dr. K. L. LOENING, Prof. M. L. MCGLASHAN; Prof. H. M. N. H. IRVING and Prof. W. KLYNE as Observers.

1. Prof. BELCHER intimated that his period of office as Chairman of Commission V.3 was now terminating and Prof. IRVING would succeed him. Accordingly, he had invited Prof. IRVING to attend as an Observer.

2. At the first meeting of the Committee in Paris in 1965, Commission V.3 had been asked to prepare a list of trivial names of reagents used in analytical chemistry. The tentative report was now ready (prepared by Prof. IRVING) and was circulated. Comments are to be sent to Prof. IRVING. Copies would be sent to the Divisions of Inorganic and Organic Chemistry to ensure that IUPAC terminology was used. Dr. LOENING would take care of this operation.

3. Prof. MCGLASHAN stated that inter-Divisional agreement was necessary between Commissions I.1, I.3, V.3, and V.5 and it was hoped that a meeting of representatives (two from each Commission) would be held in 1970. The total cost would be \$2,000 and it was asked that this cost be shared by the Divisions of Analytical and of Physical Chemistry. The purpose would be the integration of existing drafts on electrochemical nomenclature to get an agreed draft, which would appear as an Appendix to the *Manual of Symbols and Terminology for Physicochemical Quantities and Units*. This was supported unanimously and the respective Divisions would be approached.

4. The Commission on Macromolecular Nomenclature (IV.1) and the IUPAC-IUB Commission on Biochemical Nomenclature have common problems and would like to exchange Observers at meetings. The Committee supported the proposal and asked Council to support it financially.

5. The IUPAC-IUB Commission on Biochemical Nomenclature and the Commission on Nomenclature of Organic Chemistry (III.1) have exchanged Observers in the last three years, one from each Commission participating in the annual meeting of the other Commission. This exchange has been very helpful. It is desirable to put the necessary financial support on a regular basis. The Committee supported this suggestion and asked Council to make the necessary financial arrangements.

6. The Committee discussed publication at some length and finally passed the following proposal:

The Committee asks Council that all IUPAC recommendations on Nomenclature, Standards, and similar matters, whether tentative or definitive and whether or not they have already been published by IUPAC, should be freely available for publication in any language.

Prof. BELCHER dissociated himself from the motion, which was carried.

7. Prof. HOFFMANN-OSTENHOF proposed that the term Convenor be changed to Chairman, Recorder to Secretary, and that the IUPAC Secretariat should supply a Minutes Secretary for meetings of the Committee. This was agreed unanimously.

8. Prof. HOFFMANN-OSTENHOF proposed that a vote of thanks be passed to Prof. BELCHER for his services to the Committee. This was approved unanimously.

9. Prof. IRVING agreed to serve as Secretary in place of Prof. BELCHER.



## MEETING OF INDUSTRIAL MEMBERS

4th July 1969

*Present:* The meeting was attended by 59 members from IUPAC Units and National Delegations.

In his opening address, Dr. W. GALLAY (Canada) who acted as Chairman, reminded the meeting of the aims of IUPAC towards industry as stated by Lord TODD at the XXIIIrd IUPAC Conference. In this respect Dr. GALLAY questioned whether the Applied Chemistry Division was broad enough in scope.

Prof. P. W. WEST (USA) in his supporting introduction informed the meeting of a circular he had sent to industrial companies in USA. So far there had been few definite proposals as to what industry would like to see IUPAC doing in the future. In fact, many chemists within these companies had little or no idea of the present functions of IUPAC: an increased publicity of IUPAC's affairs seemed desirable.

Prof. O. WICHTERLE (Czechoslovakia), as the third member of the convenors of the meeting, stressed the need for a much closer cooperation between *pure* and *applied* chemists. This point prompted several speakers to ask for the present ratio of academic to industrial members of Commissions. Dr. R. MORF (Switzerland) thought that the ratio was about 6:1. In support of this ratio, Mr. K. M. BILLS (UK) informed the meeting that Divisions I-V (inclusive) had some 20 industrial members and Division VI had 37. Dr. F. ENGEL (Germany) felt that these figures were slightly misleading in so far as some Commissions had Working Groups in which industrial membership was high.

Whilst it was generally agreed that Commissions should try to seek a better balance in membership, the question was raised whether in fact industrial chemists had a broad enough knowledge for certain fields. Prof. J. C. BAILAR, Jr. (USA) pointed out that it was far easier for an academic to become known in a field through his publications than for an industrialist, and this perhaps contributed to the present imbalance in membership. Dr. GALLAY wondered whether Commissions should decide a programme of work and then select the most suitable chemists for the job.

In the fields of standardization and nomenclature, everyone felt that IUPAC was performing a worthwhile function. Opinion was unanimous, however, that increased publicity of the various recommendations was necessary before they might achieve universal usage. As a help towards this goal a speed-up in the time of publication would be necessary. Dr. M. WILLIAMS (UK) was able to assure the meeting that this point had already been considered by the Bureau: a new publication policy had been approved which it was hoped would meet this criticism.

For the future, Mr. M. N. DENIZTEKIN (Turkey) asked in what ways IUPAC and the smaller countries could work in greater unison. At present, some companies in such countries used the reports of IUPAC without making any financial contribution towards its organization. This was nevertheless a two-way problem and perhaps IUPAC should help more in the future development of chemistry in these countries. Prof. BAILAR drew attention to the Company Associates Plan which would partly answer Mr. DENIZTEKIN's question. He hoped that National Adhering Organizations would continue to promote and expand this Plan.

Other suggested ways in which IUPAC could assist industry were by sponsoring symposia of specific interest to them. For example, Dr. R. W. CAIRNS (USA) thought there was a need for symposia on (1) Supply of

Materials, and (2) Quality of the Environment. Dr. GALLAY reported that, in principle, the Bureau had accepted the need for such meetings and pointed out that the Applied Chemistry Division had begun preparations for a Conference on *The Role of Chemistry in Present and Future World Food Supplies*.

# PHYSICAL CHEMISTRY DIVISION COMMITTEE

1st July 1969

*Present:* Sir HARRY MELVILLE (in the chair), Prof. G. M. SCHWAB, Dr. G. WADDINGTON, Prof. Th. FÖRSTER, Prof. J. Th. G. OVERBEEK, Prof. M. PRETTRE, Dr. H. A. SKINNER, Dr. D. R. STULL.

*Apology for non-attendance:* Prof. G. EMSCHWILLER.

*In attendance:* Dr. R. N. JONES, Prof. J. JORDAN, Prof. M. L. MCGLASHAN, Mr. R. J. M. RATCLIFFE.

## I. Report on Divisional Activities

Sir HARRY MELVILLE drew attention to the Physical Chemistry Division Report which would be presented under Item 14 of the XXVth Council Meeting.

With regard to the item on nomenclature in the report of Commission I.3, Prof. JORDAN expressed concern that CITCE was also preparing nomenclature on electrochemistry. He felt that this was not one of its functions although his Commission would maintain interest in this and other relevant organizations. Commission I.3 would like to see negotiations opened with CITCE on the question of nomenclature. Sir HARRY agreed to draft a resolution to this effect for the meeting on 5th July. If approved, this resolution would be put before Council later that day.

Prof. OVERBEEK indicated that the Comité International de la Détergence was also recommending nomenclature on many aspects of colloid and surface chemistry. He felt that in this instance questions were best dealt with by the Division Committee rather than Commission I.6 because at present there was a good relationship between the two bodies.

Finally, the President reported that permission to dissolve Commission I.7 would be sought from Council.

## 2. Reports from Chairmen of Commissions

*Commission I.1*—At its meeting on 30th June the following resolution had been unanimously approved:

The International Union of Pure and Applied Chemistry strongly supports Recommendation UI (1969) of the Comité Consultatif des Unités that the mole be recognized as an SI Base Unit and urges the Comité International des Poids et Mesures to present it with full support to the XIVth Conférence Générale des Poids et Mesures.

The Division Committee endorsed this resolution, which would be put to Council and subsequently sent to the Secretary of the Comité International des Poids et Mesures.

The Commission had revised the *Manual of Symbols and Terminology for Physicochemical Quantities and Units* in the light of a further 94 comments received since its meeting in 1968 at Exeter. It was resolved that the Manual be presented to Council for approval as the final version for publication at an early date as the 'Green Book'.

Future work of the Commission would involve the compilation of Appendices to the Manual. In this respect several members stressed the importance of holding inter-Commission meetings in order to discuss the subjects involved. Sir HARRY MELVILLE reminded the meeting that proposals for such



discussions should, where possible, be presented to the Division Committee at its next meeting.

Dr. STULL envisaged that future developments in the field of nomenclature would involve the use of computerization and that this should be anticipated when preparing further reports. The Members were asked to consider this question and present their views at the next meeting.

The Committee was unanimous on the importance of achieving wide circulation of nomenclature reports especially to schools and universities. Mr. RATCLIFFE reported that this question had been discussed by the Committee on Teaching of Chemistry and appropriate action was now being taken through the Secretariat.

*Commission I.2*—Dr. SKINNER reported that the question of cost of *Experimental Thermodynamics*, Vol. I in USA and Europe had now been resolved. Butterworths had terminated its agreement with Plenum Press and Vol. II would be more consistent in price throughout the world.

*Commission I.3*—Prof. JORDAN said that the Commission would like to publish reports on

- (a) Electrochemical Thermodynamic Data
- (b) Consolidated Questionnaire on Electrochemical Kinetic Data
- (c) Guidelines for Design of Mechanistically Significant Experiments in Electrode Kinetics

in various journals rather than in *Pure and Applied Chemistry*. The President reminded the meeting that all reports from Commissions must in the first instance be offered to Butterworths for publication.

Prof. JORDAN would also like to publish an activity report on his Commission, since he felt there was a great need to publicize widely the activities of IUPAC. Other Members supported this view and it was agreed that this could be carried out without reference to the Editorial Board.

There would be a symposium in Paris, July 1970, on *Non-Aqueous Electrochemistry* which had received the support of the Division Committee and been granted IUPAC sponsorship.

*Commission I.4*—Dr. STULL said that the report *Catalog of Physicochemical Standard Substances* was nearly ready for publication. Satisfactory progress was being made on another important report *Precise Redetermination of the Density of Water*.

Other important areas in which the Commission was actively engaged were the Task Force on *Water Vapour Pressure* and a Joint Task Force with Commission I.2.

A Physical Property Task Group under Dr. KIENITZ was carrying out a search for suitable standards for calibration in all areas of physical chemistry.

A proposal from the Commission that the word 'Data' be dropped from its official title was approved by the Committee.

Prof. MCGLASHAN asked whether there might be an overlap in the work being carried out by Dr. BROWN and Prof. PLEBANSKI on *List of Terms and Units having Ambiguities that Should be Resolved* together with Dr. HERINGTON's work on *Some Problems in Physical Chemistry Created by the Use of SI Units and by Changes in Measurement Scales* and the Manual just completed by Commission I.1. It was agreed that the two Commissions should co-operate on these questions.

*Commission I.5*—Dr. JONES reported that funds had now become available from elsewhere for work to be carried out on the collection of *Rules for Retrieval of Spectroscopic Data*.

*Commission I.6*—Its role in the field of heterogeneous catalysis was to be reviewed and the possibility of setting up a Sub-Commission might be proposed.

Prof. OVERBEEK anticipated that the nomenclature report *Manual of Definitions, Terminology, and Symbols in Colloid and Surface Chemistry* would be presented at the next meeting of the Division Committee. Representatives from Commission I.1 would attend the Commission meetings, and it was hoped that the question of symbols for Helmholtz energy could be resolved.

It was suggested that the proposed investigation on *Colloid and Surface Chemistry Aspects of Environmental Science* should be discussed with appropriate Sections of the Applied Chemistry Division. Prof. OVERBEEK said this would be borne in mind when discussions took place at the Commission meeting on 3rd July.

The Commission was organizing a *Symposium on Surface Area Determination* at Bristol later this month, which had received IUPAC sponsorship.

### **3. Report on Plasma Chemistry**

Dr. SKINNER said that meetings of an *ad hoc* Committee consisting of Dr. C. W. BECKETT, Dr. L. DEFFET and Dr. V. V. SYTCHEV would take place on 1st July.

### **4. Prof. Kondratiev's Memorandum on Critical Data on Chemical Kinetics**

Dr. SKINNER reported that OSTI is supporting a data compilation report from his Commission. Dr. WADDINGTON informed the Committee that CODATA will be establishing a Task Group on Data for Chemical Kinetics under the Chairmanship of Dr. S. W. BENSON.

Before discussing this subject further the President drew attention to the fact that it was to be discussed by the Bureau on 4th July and that he would inform the Division Committee at its next meeting as to any decisions reached. However, the Committee felt that this field was so wide, especially for elementary reactions, that it would be far better for CODATA to tackle the problem.

### **5. Sponsorship of Meetings**

Mr. RATCLIFFE informed the Committee that new rules regarding IUPAC sponsorship had been agreed by the Executive Committee.

### **6. Any Other Business**

Sir HARRY MELVILLE placed a letter from Dr. W. ZATTAR (Brazil) before the Committee, mentioning that he was a candidate for election to the Bureau. The Committee was unsure as to whether Dr. ZATTAR was also interested in becoming a member of a Physical Chemistry Commission but, since his activities were not in this field, decided to take no further action.

A letter from the Romanian National Adhering Organization proposing the names of Prof. I. G. MURGULESCU and Prof. V. SAHINI for membership of the Physical Chemistry Division was also read. The Commission Chairmen present agreed to consider these names during their elections.

5th July 1967

*Present:* in addition to those present on 1st July (except for Prof. J. JORDAN) Dr. C. W. BECKETT and Prof. J. KORYTA were also in attendance.

### **I. Report of Bureau Meeting held 4th July**

Sir HARRY MELVILLE reported on the following items which had been discussed by the Bureau:

*Plasma Chemistry*—The Bureau had approved Dr. BECKETT's recommendation that a Sub-Commission of Commission I.2 be formed to deal with Plasma Chemistry. At present this unit should consist of three Associate Members: Dr. BECKETT (Chairman), Dr. L. DEFFET and Dr. V. V. SYTCHEV. Dr. BECKETT informed the Committee that as this field expanded it would probably be necessary at a future date to form a Commission on the subject. The meeting endorsed the decision to appoint a Sub-Commission.

*Chemical Kinetics*—The CODATA proposals had been discussed. It was agreed that selected Members of Commissions I.3 and I.6 should cooperate with CODATA. Other Divisions of IUPAC would similarly cooperate, *e.g.*, Macromolecular Division would send data on polymer reactions. Sir HARRY felt that although it would be preferable to have a Commission on Chemical Kinetics within the Physical Chemistry Division, it was not possible at this stage.

*Machine Documentation*—This had been discussed by the Bureau and Council would be recommended to appoint an Inter-Divisional Committee on Machine Documentation in the Chemical Field.

Prof. MCGLASHAN was sure that the new *Manual of Symbols and Terminology for Physicochemical Quantities and Units* could easily be translated into machine language and hoped that this would be a part of the future programme. He thought it was important that the subject be kept under constant review within the Division.

In view of this suggestion Dr. STULL agreed to prepare a memorandum on the subject. It was unanimously agreed that the Physical Chemistry Division should cooperate in IUPAC efforts to promote standardization of machine documentation for chemistry. Dr. JONES reminded the meeting that CODATA already had a Task Group investigating the problem.

Dr. WADDINGTON felt that it was extremely important that since the IUPAC Committee would be continuing the work, there should be a representative from the Physical Chemistry Division involved.

### **2. Reports by Commission Chairmen**

*Commission I.1*—Prof. MCGLASHAN drew attention to the fact that the Commission was proposing to hold two inter-Commission meetings in 1970, each consisting of 6-8 Members; the total budget required would be of the order of \$4,000. The meeting approved this budget and agreed to make the appropriate requests to the Treasurer.

On behalf of his Commission, Prof. MCGLASHAN asked that the Division Committee endorse the following resolution:

Commission I.1 unanimously resolved to ask the Division Committee to transmit to Council its warm appreciation of the help given to the Commission by the Secretariat both before and during the Conference.

This resolution was endorsed unanimously.



With regard to elections, it had been decided that in view of Prof. ASTACHOV's difficulty in attending meetings, one Titular Membership be left vacant until consultations with senior physical chemists in USSR had taken place.

*Commission I.2*—Dr. SKINNER asked for approval of the suggested membership of the new Sub-Commission on Plasma Chemistry. This was unanimously approved by the Division Committee.

It was proposed to hold a meeting on *Calorimetry and Experimental Thermodynamics* to be organized jointly by the Commission and the XXVIth US Calorimetry Conference, prior to the XXVIth IUPAC Conference, in the vicinity of Boston or Washington. The organizers would be seeking IUPAC-sponsorship. The Division Committee unanimously gave its support to the symposium.

No meetings would be held in 1970, though the Commission would seek an additional meeting in conjunction with the above symposium.

The Thermodynamics Tables Project under Dr. ANGUS is expected to be in a position to produce the first compilations later this year. A meeting of the Editorial Board, a representative of Butterworths, a representative of OSTI, and Dr. ANGUS would be arranged to discuss the publication procedure to be adopted.

Approval by the Division Committee for an extension of Prof. SUNNER's term as Titular Member was sought before the names were submitted to the Bureau. This was approved.

*Commission I.3*—Prof. KORYTA sought permission for publication of the report *Guidelines for Design of Mechanistically Significant Experiments in Electrode Kinetics* in electrochemical journals. The President reminded the meeting of IUPAC publications policy and said that in the first instance this should be submitted for publication in the *Information Bulletin*.

In order to clarify the position with regard to electrochemical nomenclature, a meeting between representatives of Commissions I.1, I.3, V.3, and V.5 had been proposed for 1970. This meeting had been approved by the Inter-Divisional Committee on Nomenclature and Symbols with a request to the respective Divisions for endorsement. The Physical Chemistry Division Committee endorsed this request.

A suggestion that approaches be made to the IUPAC Treasurer for a salaried scientific assistant to aid Prof. MILAZZO in the preparation of Electrochemical Thermodynamic Data was withdrawn after a brief discussion.

It was hoped to complete the report on Electrochemical Kinetic Data in time for publication by 1971.

The *Symposium on Non-Aqueous Electrochemistry* has requested financial support from IUPAC of \$1,000. A meeting of the Commission is scheduled to take place for two days during the symposium, and the budget will be approximately \$2,000.

The relationship between the Commission and CITCE is now satisfactory, CITCE having agreed that, in future, electrochemical nomenclature will be the responsibility of Commission I.3. CITCE will function solely as an international society.

*Commission I.4*—The monograph on *Characterization of Chemical Purity—Organic Compounds* is nearing completion.

The report prepared by Drs. MASHIKO, PLEBANSKI, and STULL on *Catalog of Physicochemical Standard Substances* was submitted for approval by the Division Committee for publication. This was carried unanimously.

It is planned to hold a meeting of the Physical Property Task Group at Ludwigshafen in June 1970. A grant of \$1,000 towards the expenses is requested, the remainder of the funds being provided by Badische Anilin- und Soda-Fabrik AG. Sir HARRY MELVILLE agreed to draw the attention of Council to the close liaison established with industry by this Task Group.

Since the data activities of the Commission had declined to zero, it had been decided to change the title to *Commission on Physicochemical Measurements and Standards*. This title was approved by the Division Committee.

Dr. STULL expressed concern over the non-participation of elected Members from USSR. Other Members agreed with this point and the President agreed to raise the matter at the meeting of Division Presidents on 6th July.

*Commission I.5*—The Commission had completed its report on *Tentative Recommendations for Presentation of NMR Data for Publication in Chemical Journals*, the publication of which was approved by the Division Committee.

*Commission I.6*—Prof. OVERBEEK reported that agreement had been reached with Commission I.1 as to the symbol to be used for Helmholtz energy. Other amendments to the *Manual of Definitions, Terminology, and Symbols in Colloid and Surface Chemistry* had also been incorporated in the version to be presented to Council. The Division Committee approved this Manual for tentative publication.

The Commission proposes to extend its activities in the field of heterogeneous catalysis. In order to make this effective a request for enlargement to 9 Titular and 10 Associate Members was made and approved by the Division Committee. Dr. Waddington undertook to place the matter before the Bureau.

Activities in the field of education would be extended. A Task Group had been formed to investigate the production of a work-textbook for colloid and surface chemistry and also the production of film loops. Close cooperation with the Committee on Teaching of Chemistry would be maintained on these topics.

With the nomination of Prof. LANGE as Associate Member, satisfactory liaison with Comité International de la Détérgence will be continued.

Since Prof. Everett will take over as Chairman, the Commission asked that his name be placed before the Bureau as the official representative of IUPAC on the International Congress on Catalysis.

(The meeting adjourned until 6th July for consideration of the remaining item on the agenda.)

### **3. Election of President, Secretary, and Members of Division Committee**

It was unanimously agreed that a letter be sent to the retiring Secretary, Prof. EMSCHWILLER, thanking him for his services to the Physical Chemistry Division: Sir HARRY MELVILLE to act.

Further discussion on the nomination of Members from USSR took place and it was decided that for the period 1969-71, Dr. V. I. VEDENEV be elected an Associate Member of the Division Committee. The following Titular Members were then elected:

Dr. G. WADDINGTON (President), Sir HARRY MELVILLE (Past-President), Prof. J. Th. G. OVERBEEK (Vice-President), Dr. R. N. JONES (Secretary), Prof. E. U. FRANCK, Prof. J. JORDAN, Prof. M. L. MCGLASHAN, Prof. M. PRETTRE, Dr. D. R. STULL, Prof. S. SUNNER.

## COMMISSION I.1: PHYSICOCHEMICAL SYMBOLS, TERMINOLOGY, AND UNITS

### 1. Meetings

Two meetings of the Commission have been held since 1967, one at Exeter on 19th and 20th December 1968, and the other at Cortina d'Ampezzo on 30th June and 1st and 2nd July 1969. Titular Members attending were McGLASHAN, PAUL, BATES, FAYARD (Cortina only), JAENICKE (Cortina only), JELLINEK (Exeter only), PEREZ-MASÍÁ, and SILLÉN. Associate Members SEKI and WADINGTON attended the Cortina meeting.

### 2. Manual

Following the publication of the tentative version of the *Manual of Symbols and Terminology for Physicochemical Quantities and Units* in *Information Bulletin* No. 32, more than 200 pages of comments were received and considered by the Commission. The Manual, revised in the light of these comments, was approved by Council on 7th July for definitive publication.

### 3. Appendices

Commission I.1 does not contemplate an early beginning to the work of preparing a successor to the present Manual, believing that it should now be allowed to remain undisturbed at least for several years. Instead, the Commission has begun work on a project for attachment to the Manual of a number of Appendices dealing in detail with specialized fields of physical chemistry. One such Appendix on *Definition of Activities and Related Quantities* has been included in the present Manual and will it is hoped serve as a model for future ones. These Appendices will be prepared by collaboration with other Commissions. Following correspondence, and fruitful discussions at Cortina, with Commissions I.2 (Thermodynamics and Thermochemistry), I.3 (Electrochemistry), I.5 (Molecular Structure and Spectroscopy), and I.6 (Colloid and Surface Chemistry), the preparation of Appendices has been initiated in each of these four fields, in which the need seems most urgent.

### 4. Resolution Concerning the Mole

The Commission unanimously recommended that Council approve the following resolution and send it to the Secretary to the Comité International des Poids et Mesures:

The International Union of Pure and Applied Chemistry strongly supports Recommendation U1 (1969) of the Comité Consultatif des Unités that the mole be recognised as an SI Base Unit, and urges the Comité International des Poids et Mesures to present it with full support to the XIVth Conférence Générale des Poids et Mesures.

This resolution was unanimously approved by Council on 5th July.

### 5. Membership

The term of appointment of only one Titular Member (K. V. ASTACHOV) expired at the Conference. It was resolved to leave the position vacant in the meantime, and to fill it by postal ballot after consultations with senior physical chemists in USSR. Dr. J. TERRIEN, Director of the International Bureau of Weights and Measures, was nominated as a new Associate Member.



## COMMISSION I.2: THERMODYNAMICS AND THERMOCHEMISTRY

1. The Commission met on four occasions during the period 2nd-4th July, 1969. The following members attended during these meetings: BECKETT, FRANCK, GERASSIMOV, ROSSINI, SEKI, SKINNER, SUNNER, VODAR (Titular Members); COLOMINA, DEFFET, MCGLASHAN, NEWITT, SCHAFER, WADDINGTON, WADSÖ, WESTRUM (Associate Members); ANGUS, HERINGTON, STULL (Observers).

2. The implications of recent changes in the International Practical Temperature Scale, in the value of the volt, and in the Pressure Scale were discussed. Prof. ROSSINI was asked to prepare a brief report on the effects of the changes in the Temperature Scale in respect of thermodynamic measurements, to be offered for publication in *Pure and Applied Chemistry* and in *J. Chem. Thermodynamics*. The changes in the Pressure Scale are to be reprinted in *Bulletin of Thermodynamics and Thermochemistry*.

3. Prof. SUNNER agreed to write to selected experts on the measurement of pressure to enquire if agreement can now be reached by writing and meeting amongst themselves to formulate an International Practical Pressure Scale up to limits of ca. 20 k.bar ( $2.10^8$  Pascal).

4. It was reported that the *International Conference on Thermodynamics* (Cardiff, April 1970) is to be sponsored by IUPAC.

5. It was agreed to request IUPAC sponsorship of a joint meeting on *Calorimetry and Experimental Thermodynamics* with the XXVth US Calorimetry Conference, to be held at a location convenient to Washington, DC in the week prior to the XXVth IUPAC Conference at Washington (July 1971).

6. Dr. BECKETT reported that the *ad hoc* Committee (BECKETT, DEFFET, SYTCHEV) on Plasma Chemistry would request of the Bureau:

- (a) that a Sub-Commission on Plasma Chemistry be formed, and
- (b) that funding be given to organize a small *Symposium on Plasma Chemistry* to be held in Washington, DC in July 1971.

7. Prof. WESTRUM reported on the growth of *Bulletin of Thermodynamics and Thermochemistry*. Sales have reached 600 copies/annum, and the latest issue has 594 pages. The *Bulletin* is now without subvention; this, coupled with the increasing size of each issue, has necessitated a price increase to \$12/issue. The Editor asked permission of the Commission

- (a) to add new members to the Editorial Board, and
  - (b) to change the title to *Bulletin of Chemical Thermodynamics*.
- The Commission agreed.

Discussion followed on the desirability of a similar change in title of Commission I.2. Opinions were divided and no change is to take place at this time.

8. *Experimental Thermodynamics*, Vol. II (in preparation), was discussed in relation to the price structure imposed on *Experimental Thermodynamics*, Vol. I by Plenum Press in respect of sales in USA. The Chairman reported that Butterworths will act as US distributors after July 1969, and that the American price structure for Vol. II will not be unreasonable relative to UK price. In the light of this assurance, it was agreed that Vol. II be offered to Butterworths when completed. Prof. VODAR stated that progress on Vol. II should speed up this year.

9. Prof. NEWITT reviewed the status of the Thermodynamic Tables Project Centre. The tables on Ar, CO<sub>2</sub>, and O<sub>2</sub> are well advanced, and it is

anticipated that the Ar tables will be completed at the end of 1969. It was stressed in discussion that information on the progress of Tables should be widely disseminated, preferably by the issue of brief newsletters.

The question of publication policy was raised. It was agreed that a policy, satisfactory to the various national financial sponsors, for publication of the skeleton and extensive Tables originating from the Centre be sought by the Director in consultation with the IUPAC Editorial Board and Butterworths.

10. Prof. McGLASHAN requested on behalf of Commission I.1 that Commission I.2 cooperates in the preparation of an Appendix to the new *Manual of Symbols and Terminology for Physicochemical Quantities and Units*, and that this Appendix deals specifically with thermodynamic quantities. It was agreed to set up a Working Party of 3 Members from Commission I.2 to collaborate with a similar Working Party from Commission I.1.

11. Dr. STULL requested on behalf of Commission I.4 that a Working Party of 3 Members from Commission I.1 be set up to collaborate with a similar Working Party from Commission I.4 to examine selected standard reference materials for calibration purposes in experimental thermodynamics, which was agreed.

12. Prof. ROSSINI and Dr. WADDINGTON reported on CODATA activities. Prof. SUNNER outlined progress made by the joint IUPAC-CODATA Task Group on Key Values for Thermodynamics. It was agreed to leave this project under the control of CODATA but to maintain collaboration with Commission I.2.

13. Reports on Calorimetry Conferences in Japan (SEKI), UK (SKINNER), USA (WADDINGTON), and USSR (GERASSIMOV) were presented. The *1st International Calorimetry Conference* (Warsaw, 1969) was reported to have attracted 150 papers and some 400 participants.

14. Prof. McGLASHAN outlined aspects of the practical usage of SI Units.

## COMMISSION I.3: ELECTROCHEMISTRY

### 1. Meetings

Meetings were held on three consecutive days, viz. 2-4th July. The following members attended: BATES, EPELBOIN, HAASE, JORDAN, KORYTA, MILAZZO, TAMAMUSHI (Titular Members); BRUSSET, DEFAY, LEVART, VALENSI, VAN RYSELBERGHE (Associate Members); PIONTELLI (National Representative).

### 2. Minutes

The minutes of the preceding meeting, held in Detroit in September 1968, were ratified.

### 3. Projects Completed

Prof. JORDAN and Dr. TAMAMUSHI were authorized to finalize *Guidelines for Design of Mechanistically Significant Experiments in Electrode Kinetics*. The Division Committee will be requested to authorize publication in electrochemical journals, and possibly in the *Information Bulletin*.

### 4. Projects in Progress

(a) *Electrochemical Nomenclature*. A document entitled *Sign Conventions Concerning Galvanic Cells and Electrodes* had been circulated in advance of the Conference. Two alternative sets of nomenclature recommendations, identified as TEXT I and TEXT II had been offered. The following resolution was adopted:

Commission I.3 endorses in substance the Stockholm Convention as formulated in the IUPAC *Manual of Symbols and Terminology for Physicochemical Quantities and Units* with the expectation to clarify and extend it in appropriate Appendices. Consequently, Commission I.3 does not endorse at this time the terminology introduced in TEXT I and TEXT II.

The Chairmen and Secretaries of Commissions I.3 and V.5 had met with the Chairman of Commission I.1 and discussed the preparation of an Appendix devoted to cells under flow of a finite current. Commission I.3 will focus attention on relevant physicochemical quantities and Commission V.5 on methodologies. It is expected that these efforts will be coordinated at an *ad hoc* meeting of representatives of Commissions I.1, I.3, V.3, and V.5 sometime in 1970. The matter has been referred to the Inter-Divisional Committee on Nomenclature and Symbols.

(b) *Electrochemical Thermodynamic Data*. Compilations of electrode potentials by Prof. MILAZZO were reviewed. A comprehensive set of tables is expected to be ready for publication in 1971. This project is being coordinated with Commission V.5 under whose auspices a *critical* (rather than comprehensive) tabulation of data on selected systems in aqueous solutions is being submitted for publication by Prof. CHARLOT. Cooperation for coordinating the two projects was the subject of two meetings between the Chairmen and Secretaries of Commissions I.3 and V.5 on 1st and 4th July. Minutes of these meetings (recorded by Dr. ZUMAN) are published separately in the *Comptes Rendus* (see p. 85).

(c) *Electrochemical Kinetic Data*. A questionnaire drafted by Dr. TAMAMUSHI and Prof. TANAKA was approved. It will be distributed to authors of papers



on electrode kinetics, in order to obtain requisite information for an updated edition of the *Tables of Kinetic Parameters* published in 1964. The tentative target date for completion of this project is 1971.

(d) *Symposium on Non-Aqueous Electrochemistry* (co-sponsored by Commissions I.3 and V.5). Plans were approved for holding the symposium in Paris, between 6th and 11th July, 1970. The tentative programme included 7 plenary lectures, 14 invited talks, and 30 short communications. Members of Commission I.3 will send suggestions on speakers and topics to the Executive Chairman of the Local Arrangements Committee (Dr. J. BADOZ).

(e) *Meeting of Commission I.3 in 1970*. A plenary meeting has been scheduled in Paris to expedite projects in progress, with a view to completing significant assignments (in the areas of nomenclature, electrochemical thermodynamics, and kinetics).

## 5. Relations between IUPAC and CITCE

These have been satisfactorily normalized. It is understood that matters of electrochemical nomenclature are the concern of Commission I.3 which will cooperate fully with Commission I.1. CITCE will function as an international society of electrochemistry which organizes scientific meetings. CITCE will *not* publish any nomenclature proposals under its auspices.

## 6. Elections

(a) It was resolved that:

Commission I.3 will not ask for any exceptions to extend memberships beyond 8 years (without prejudice to currently continuing terms).

(b) The Commission was reconstituted as follows: Prof. J. JORDAN (Chairman), Prof. A. N. FRUMKIN (Vice-Chairman), Prof. J. KORYTA (Secretary), Dr. I. EPELBOIN, Prof. R. HAASE, Prof. G. MILAZZO, Dr. A. SANFELD, Dr. R. TAMAMUSHI (Titular Members); Prof. V. S. BAGOTZKY, Prof. H. BRUSSET, Prof. H. GERISCHER, Dr. W. J. HAMER, Dr. E. LEVART, Dr. R. PARSONS, Dr. H. TANNENBERGER, Prof. E. YEAGER (Associate Members); Prof. L. ERDEY-GRÚZ, Prof. R. PIONTELLI, Prof. S. MINČ (National Representatives). Enquiries will be made to ascertain the continued availability as National Representatives of Prof. M. KARSULIN and Prof. A. RUIS-MIRO.

## Joint Meetings of Chairmen and Secretaries of Commissions I.3 and V.5

The Chairmen and Secretaries of Commissions I.3 and V.5 met on 2nd and 4th July. The Chairman of Commission I.1 was present at the second meeting.

The progress in the preparation of the jointly sponsored *Symposium on Non-Aqueous Electrochemistry* to be held in Paris during 6-11th July, 1970, was reviewed.

On nomenclature the meeting was informed that Commission I.3 endorsed the Stockholm Convention. TEXTS I and II were rejected. The IUPAC *Manual of Symbols and Terminology for Physicochemical Quantities and Units* will be supplemented by publication of Appendices on special topics. First drafts of the proposal of terms for selected topics (Commission I.3) and techniques (Commission V.5) should be available before January 1970. An inter-Commission meeting of representatives of Commissions I.1, I.3, V.3, and V.5 will be held during 1970.

The sample of compilation of oxidation-reduction potentials collected by Prof. G. MILAZZO will be submitted to all members of Commissions I.3 and V.5 with a request for comments and criticism. Any comments should be sent directly to Prof. MILAZZO with copies to the Secretaries of Commissions I.3 and V.5. The request by Commission I.3 for financial support is supported by Commission V.5. A request was made that several copies of the report by Prof. G. CHARLOT on selected values of oxidation-reduction potentials should be made available to Commission I.3. If the report by Prof. MILAZZO is published before the report by Prof. CHARLOT, permission from Prof. CHARLOT should be obtained for the publication of those data which were taken from the report by Prof. CHARLOT. Prof. MILAZZO suggested that he and Prof. CHARLOT should be present at all inter-Commission meetings at which the problem of tables of oxidation-reduction potentials is discussed.

The scope of the division of the work on projects on electrochemistry in non-aqueous media will be discussed at Paris, July 1970.

The report by Prof. N. TANAKA on pretreatment of solid electrodes should be distributed to the members of Commission I.3 with the request for comments and criticism to be sent to Prof. TANAKA with copies to Dr. ZUMAN.

The programmes of both Commissions are to be published jointly in journals suggested by the two Commissions, e.g., *J. Electroanal. Chem.*, *Anal. Chem.*, *J. Electrochem. Soc.*, *Analyst*, *J. Electrochem. Soc. Japan*, *Japan Analyst*, *J. Chim. phys.*, *Chem. and Eng. News*, *Chem. in Britain*, *Angewandte Chem.*, *Chem. listy*, *Electrochimija*. Permission should be given for reprinting in any other journal in the world.

## COMMISSION I.4: PHYSICOCHEMICAL MEASUREMENTS AND STANDARDS

1. The Commission met on three occasions during the period 1st-3rd July. The following members attended during these meetings: STULL, HERINGTON, BROWN, KIENITZ, MASHIKO, MEINKE, PLEBANSKI (Titular Members); FRANC, STAVELEY, SUNNER (Associate Members); FEUERBERG, GRAHAM, MILONE, SMIT (National Representatives); TERRIEN, WADDINGTON (Observers).

2. The Commission made the following nominations:

(a) *Titular Members*. Re-elected for 1969-1973—Dr. I. BROWN, Dr. W. W. MEINKE. Elected for 1969-1973—Dr. J. FRANC.

(b) *Associate Members*. Re-elected for 1969-1971—Dr. L. A. K. STAVELEY, Prof. S. SUNNER. Elected for 1969-1971—Dr. J. P. CALI, Dr. A. JUHASZ, Prof. W. SIMON.

The Commission hopes that Dr. T. PLEBANSKI will be invited to serve as a National Representative on this Commission.

3. Dr. SAYLOR sent word that the report of the *Ottawa Purity Symposium* is nearly complete.

4. Dr. STAVELEY reported on the monograph *Characterization of Chemical Purity-Organic Compounds*. All the manuscripts except that on Raman spectroscopy have been edited. A draft preface prepared by Dr. STAVELEY was accepted by the Commission, which agreed that a summarizing chapter or table was unnecessary.

5. The *Catalog of Physicochemical Standard Substances*, prepared by Drs. MASHIKO, PLEBANSKI, and STULL, was discussed by the Commission. It was agreed to omit radioactivity standards, and to accept modifications and additions until 1st September, 1969. To invite comment and encourage additions, this document will be published in tentative form in the *IUPAC Information Bulletin*.

6. Dr. SMIT reported briefly on the activities of the Rheology Panel of the Institute of Petroleum, and agreed to keep this Commission informed.

7. Dr. PLEBANSKI presented a memorandum by himself and Dr. STULL on the importance of a precise redetermination of the density of water. The present density of water is based on 70-year old data discordant in the sixth decimal place. Desirability of modern redetermination and the formidable problems involved were widely recognized. Dr. Terrien stated that his laboratory is studying changes in density due to changes in isotopic composition. It was reported that Dr. H. BOWMAN of US National Bureau of Standards has perfected an interferometric method for determining the volume of a steel ball later used for hydrostatic weighing experiments. An accuracy sufficient to resolve present uncertainties is claimed. Dr. STULL will enquire further into this matter.

8. Drs. BROWN and PLEBANSKI discussed possible ambiguities in the use of terms and units, but in view of the revised Manual submitted to the Conference by Commission I.1, it seemed advisable for Commission I.4 to comment during the coming year. Queries from this Commission should be transmitted to Commission I.1 through Dr. BROWN.

9. Drs. MASHIKO and SMIT reported that the Organization for Economic Cooperation and Development (OECD) does not have immediate plans for a standard materials bank.



10. Dr. WADDINGTON reported on the activities of CODATA. Because CODATA has set up a Task Group on Chemical Kinetics, it will not be necessary for Commission I.4 to deal with this subject. CODATA has also established a Commission whose object is the collection and evaluation of data for several disciplines, including physical chemistry. This induced a discussion of the data activities of Commission I.4 (these have declined to zero during the past score of years) and consideration of the deletion of the word 'Data' from the Commission's title (see Item 18 below).

11. Dr. GRAHAM presented correspondence from Dr. H. G. McADIE, Chairman, Committee of Standardization of the International Confederation for Thermal Analysis, pointing out the paucity of standards for thermal analysis. The importance of thermal analysis was recognized, as well as the desirability of establishing appropriate standards. It was agreed that members of the Commission should maintain close contact with Dr. McADIE; Dr. GRAHAM agreed to chair a liaison group including Drs. HERINGTON, SMIT, and STULL.

12. Dr. SMIT pointed out the need to agree on standard conditions for reporting numerical values of measured physicochemical properties. He agreed to prepare a paper for the 1971 meeting, including changes in measurement systems and the adoption of SI Units.

13. Dr. HERINGTON presented a memorandum entitled *Some Problems in Physical Chemistry Created by the Use of SI Units and by Changes in Measurement Scales*. The Commission agreed on the necessity of including the mole in the fundamental units defined by the General Conference on Weights and Measures (CGPM). Dr. TERRIEN urged Commission members to persuade their governments to instruct their representatives to CGPM to adopt the mole.

14. Commission I.2 has requested close liaison with Commission I.4 regarding standards of common interest. Commission I.4 welcomes the opportunity to cooperate, and to avail itself of the expertise resident in Commission I.2.

15. Dr. STULL presented the discordance in the vapour pressure of water amounting to 75 ppm. The usefulness of water as a vapour pressure standard and the need for a definitive set of tabulated vapour pressure-temperature values for water were pointed out. Dr. HERINGTON referred to the National Physical Laboratory's interest in the subject (Dr. D. AMBROSE), and welcomed the suggestion for discussions with knowledgeable individuals on the preparation of a set of definitive tables. It was agreed that Dr. STULL should act on behalf of Commission I.4 in an effort to clarify this problem.

16. The Commission unanimously expressed appreciation of Dr. STULL's historical review of the Data and Standards Commission since its foundation in 1920.

17. Following the Prague meeting, Prof. Kienitz proposed the formation of a Physical Property Task Group. The task is to suggest and examine reference substances whose constants are known with sufficient accuracy and can be used in relative measurement as reference values or for calibrating measuring equipment. Correspondence indicated sufficient support to undertake the task. Approval for the formation of this Task Group was granted by the Executive Committee of IUPAC (31st October, 1968).

Prof. KIENITZ agreed to chair this Task Group, and listed 27 separate properties germane to physical chemistry and the relative importance of each.

The Commission decided that the project should be called *Task Group on Standard Calibration Substances*. The procedure adopted for the Task Group included the following steps:

(a) Interested Members having expertise in a given physical property will write to Prof. KIENITZ informing him of their areas of interest.

(b) The Member will carry out a literature search, and will then perhaps be able to recommend a calibration standard (from already existing standards), or to propose a suitable substance for further study. If laboratory work is required, a cooperating laboratory will be sought. If suitable measurement methods are not available, collaboration with experts will be sought.

(c) Prof. KIENITZ will collect and edit the written efforts of the participants, and circulate progress reports to the Commission at semi-annual intervals.

(d) The Commission will select materials proposed as a result of studies in (b) above and recommend their use as standards.

(e) To expedite this project, it is proposed to have a meeting of major participants in Ludwigshafen, Germany, in June 1970. Accordingly, Dr. STULL has made application for a grant of \$1,000 from IUPAC funds partially to defray expenses.

(f) The Commission recognizes that expertise exists in several IUPAC Commissions that will be contributory to the success of this project, hence joint working parties will be established with the appropriate Commissions.

18. Due to the action of CODATA noted in Item 10 above, the Commission decided to replace the word 'Data' in the Commission's title with the word 'Measurements'. The terms of reference of the Commission on Physicochemical Measurements and Standards are to be the same as the Commission on Physicochemical Data and Standards, namely:

The Commission on Physicochemical Measurements and Standards strives to promote and encourage (a) the improvement and standardization of methods for measuring the physical properties of pure substance, (b) the use of standard substances for calibrating and checking in physicochemical measurements, and (c) collaboration and accord between various national organizations and institutions, whose objectives are as defined by (a) and (b) (adopted August 1953, see *Comptes Rendus XVII Conference*).

The name *Commission on Physicochemical Measurements and Standards* is to be effective from 5th July, 1969.

## COMMISSION I.5: MOLECULAR STRUCTURE AND SPECTROSCOPY

1. 2nd and 3rd July, 1969. The following were present: JONES, COLE, FÖRSTER, MILLER, MORINO, SHEPPARD (Titular Members); URBANSKI (National Representative).

Titular Member ELYASHÉVICH was delayed by travel difficulties; this prevented him from participating in the Meeting, but he subsequently expressed his full approval of all the items of business.

2. The Chairman reported that the ICSU Inter-Union Commission for Spectroscopy had been active in dealing with problems in the spectroscopic field arising from introduction of the SI Unit System. The status of the ångström has been satisfactorily clarified, and it has been clearly established that the  $\text{cm}^{-1}$  is an SI unit. Discussions at the Cortina Conference between Commissions I.1 and I.5 helped to clarify a number of other definitions in the sections of the *Manual of Symbols and Terminology for Physicochemical Quantities and Units* concerning spectroscopy. Commission I.5 endorses the comment, relevant to the ångström, which is made by Commission V.4 under Section 2.8 of its report *Nomenclature, Symbols, Units, and Their Usage in Spectrochemical Analysis-I*.

3. (a) As a result of a cooperative study in laboratories in Canada, Japan, and USA the Sub-Commission on Infrared and Raman Spectroscopy can now recommend a set of wavenumbers for the calibration of infrared spectrometers in the range  $600\text{--}300\text{ cm}^{-1}$ . A technical paper dealing with this will be submitted for publication in *Pure and Applied Chemistry*. It was also agreed that a further publication dealing with the range  $300\text{--}20\text{ cm}^{-1}$ , together with a study of higher resolution calibration data for the range  $600\text{--}20\text{ cm}^{-1}$ , should be prepared. Experimental work for this has largely been completed and will be discussed at the Technical Sessions of the Sub-Commission to be held at Sydney (August 1969).

(b) The Commission has received from the Office of Standard Reference Data of US National Bureau of Standards a technical report on improvements in the technique of Raman spectroscopy resulting from the use of laser sources. This will be considered by the Sub-Commission on Infrared and Raman Spectroscopy at the Sydney Meeting.

4. The Sub-Commission on Storage and Retrieval of Spectroscopic Data has published *Tentative Specifications for the Measurement and Evaluation of Infrared Spectra for Documentation Purposes* (Information Bulletin No. 34). Information relating to the cost and practicability of producing spectra conforming with these specifications will be forthcoming as a consequence of experiments now in progress in both academic and industrial laboratories.

5. The Commission has completed *Tentative Specifications for the Presentation of NMR Spectra for Publication in Chemical Journals*. These will be submitted to the Secretariat for publication.

6. It has been suggested to the Commission that it examines the need for uniform specifications for nomenclature, symbolism, and presentation of photoelectron spectra and of Mössbauer spectra. The opinions of several spectroscopists active in these fields have been canvassed and these subjects will be considered further when the Commission meets in Sydney.

7. The Commission has received a proposal recommending clarification of concepts related to polarizability. It will consult with experts in the field concerning the advisability of recommending changes in current practice.



8. The composition of the Commission for the period 1969-1971 was considered and the following recommendations were made:

(a) *Titular Members*. Dr. R. N. JONES (Chairman), Prof. A. R. H. COLE (Vice-Chairman), Prof. F. A. MILLER (Secretary), Dr. M. A. ELYASHÉVICH, Prof. Th. FÖRSTER, Prof. A. HADNI, Prof. Y. MORINO, Prof. N. SHEPPARD.

(b) *Associate Members*. Prof. E. FLUCK, Prof. E. R. LIPPINCOTT, Prof. R. C. LORD, Prof. S. NAGAKURA, Dr. J. PLIVÁ, Sir HAROLD THOMPSON, Dr. D. W. TURNER.

(c) *Advisory Counsellor*. Dr. G. HERZBERG.

(d) *National Representative*. Prof. T. URBANSKI.

(e) *Sub-Commission I.5.1: Infrared and Raman Spectroscopy*. Prof. R. C. LORD (Chairman), Prof. A. R. H. COLE, Prof. B. L. CRAWFORD, Jr., Prof. A. HADNI, Dr. R. N. JONES, Prof. M. L. JOSIEN, Prof. E. R. LIPPINCOTT, Prof. J. M. MILLS, Dr. G. R. WILKINSON.

(f) *Sub-Commission I.5.2: Storage and Retrieval of Spectroscopic Data*. Dr. R. N. JONES (Chairman), Dr. D. R. LIDE, Jr., Dr. A. SAVITZKY, Prof. T. SHIMANOUCI, Sir HAROLD THOMPSON.

## **COMMISSION I.6: COLLOID AND SURFACE CHEMISTRY**

### **1. Meetings**

The Commission convened on 2nd, 3rd, and 4th July. The meetings were attended by OVERBEEK, EVERETT, VAN OLPEN, BRUNAUER, KAMIENSKI, PRETTRE, SCHAY (Titular Members); BURWELL, HAUL, RIDEAL (Associate Members); and by Prof. H. LANGE (Observer for Comité International de la Détergence).

Part of the session on nomenclature was attended by Prof. M. L. MCGLASHAN, Chairman of Commission I.1, and three other Members of that Commission. The session on educational activities was attended by Prof. G. M. SCHWAB, representing the Committee on Teaching of Chemistry.

### **2. Tentative Manual of Definitions, Terminology, and Symbols in Colloid and Surface Chemistry**

A draft for this Manual had been circulated among the past and present members of the Commission. Amendments to this draft which were formulated during the meetings have been incorporated. One of these amendments, discussed with the Chairman and Members of Commission I.1 was the choice of  $A_s$  as the symbol for surface area in those cases where confusion with  $A$  for Helmholtz energy would occur. Most of the amendments were of an editorial nature, some had a technical character. In the Council Meeting of 7th July, approval was obtained for publication of the amended tentative Manual.

### **3. Nomenclature for Zeolites and Molecular Sieves**

The Commission decided to take the initiative in constituting a Working Group to deal with nomenclature of zeolites (both natural and synthetic) and molecular sieves. In the Working Group persons representing Commission II.2, as well as the International Mineralogical Association and the International Crystallographic Union, will be invited.

### **4. Activities in the Area of Catalysis**

On the initiative of the President of IUPAC the Commission decided to expand its activities in the area of catalysis. In the next two years a tentative nomenclature manual covering catalysis will be composed, the possibilities of making standard reference materials for catalysis will be considered, and symposia in the periods between International Congresses on Catalysis (ICC), covering either a limited aspect of catalysis or intended for limited regional groups, may be sponsored and initiated. The Commission extended its membership in the area of catalysis. Representatives for liaison with ICC (Prof. EVERETT) and with the Task Group on Chemical Kinetics of ICSU-CODATA (Prof. SCHUIT) were nominated.

### **5. Educational Activities**

The Commission is concerned about the general deficiency of teaching of colloid and surface chemistry at the college level in view of the great demand of industry for persons trained in these areas. As one possible approach to improve this situation the Commission agreed to the creation of a work-textbook in the form of a resource manual, intended mainly for teachers of physical chemistry courses, containing attractive experiments as well as

theoretical presentations in the fields of colloid and surface chemistry relevant to the most important topics of physical chemistry. An Editorial Committee was appointed.

The Editorial Committee was also charged with the task of exploring the possibility of preparing a catalogue of available films and film loops dealing with colloid and surface chemistry, and of making an evaluation of existing material.

## **6. Environmental Science**

Realising that the majority of problems of environmental science and pollution of air and water contain aspects of colloid and surface chemistry, the Commission wishes to make it known that it is interested in this area, and that it is anxious to cooperate with other units of IUPAC as well as outside organizations dealing with environmental science.

## **7. Symposia**

The Commission has taken the initiative for a *Symposium on Surface Area Determination* which is to be held in Bristol in July 1969, sponsored jointly by the Commission and by the Colloid and Surface Chemistry Group of the Society of Chemical Industry (UK).

The Commission considers that a symposium on colloid and surface chemistry aspects of air and water pollution would be useful and timely.

## **8. Liaison with Comité International de la Détergence**

Liaison with CID has been satisfactory in the past, and the nomination of Prof. LANGE as an Associate Member of the Commission is expected to intensify the cooperation with CID.

## **9. Membership**

On account of the 8-year rule, Titular Members Akad. M. M. DUBININ, and Profs. B. KAMIENSKI and J. Th. G. OVERBEEK were not reappointed. Prof. D. H. EVERETT was nominated as Chairman, Prof. S. BRUNAUER as Vice-Chairman, Prof. H. VAN OLPHEM remains Secretary. The Associate Members Prof. R. L. BURWELL, Prof. R. HAUL, and Dr. K. J. MYSELS have been nominated as Titular Members and with the approval of the Bureau, Prof. V. V. KAZANSKY has been nominated as a ninth Titular Member. The Associate Members Prof. G. K. BORESKOV, Prof. J. HORIUTI, Sir ERIC RIDEAL, and Prof. A. SHELUDKO remain on the Commission and the following new Associate Members have been nominated: Prof. R. M. BARRER, Prof. S. FRIBERG, Prof. H. LANGE, Prof. G. A. SCHUIT, Prof. C. KEMBALL, Prof. A. V. KISELEV.



# INORGANIC CHEMISTRY DIVISION COMMITTEE

4th July 1969

*Present:* Prof. J. BÉNARD (in the chair), Prof. O. GLEMSE, Prof. R. COLLONGUES, Prof. V. GUTMANN, Prof. K. A. JENSEN, Prof. G. SARTORI, Prof. P. SPACU, Dr. E. WICHERS.

*Apologies for non-attendance:* Prof. J. H. DE BOER, Sir RONALD NYHOLM.

## I. Survey of Commissions

The Division Committee discussed and approved the reports of the different Commissions presented by Dr. WICHERS (Chairman of Commission II.1), Prof. JENSEN (Chairman of Commission II.2), Prof. COLLONGUES (Secretary of Commission II.3).

The Division Committee approved the following modifications in the membership of the Commissions:

*Commission II.1.* Dr. WICHERS was retiring from the Chairmanship: the new Chairman is Prof. GREENWOOD (UK). Dr. GUÉRON was retiring from the Secretaryship: the new Secretary is Mr. PEISER (USA). Two new Titular Members are appointed in place of Drs. WICHERS and GUÉRON who have reached the completion of their membership period: Dr. A. E. CAMERON (USA) and Prof. E. ROTH (France).

*Commission II.2.* The Chairman of the Commission requested that the membership of all present Titular Members be renewed for a period of 2 years.

*Commission II.3.* Taking into consideration its present activity and its future plans, the Commission strongly wished the number of its Titular Members to be increased from 4 to 6. Having reached the date of completion of his membership, Prof. NOWOTNY was retiring from the Chairmanship of the Commission. Having reached the date of completion of his membership, Prof. COLLONGUES was retiring from the Secretaryship and Prof. FLOOD now also at the end of his membership leaves the Commission. Dr. HORTON (USA) was proposed unanimously as Chairman and Prof. G. D. RIECK (Netherlands) as Secretary (1969-1973). The following were proposed as Titular Members for the period 1969-1973: Prof. C. B. ALCOCK (UK), Prof. COLLONGUES, Prof. E. FITZER (Germany), and either Prof. A. E. SHEINDLIN or Prof. L. V. GURVICH (USSR).

## 2. Position of High Temperatures and Refractories Commission

The Division Committee approved the increase from 4 to 6 in the number of Titular Members of Commission II.3 and provided that Council accepts it, approved the choice of the 6 Titular Members.

## 3. Eventual Creation of a Section on Coordination Chemistry

The Division Committee considered favourably the creation of a Section composed of a limited number of members, who would study the problems of coordination chemistry and who could take part in the decisions concerning the organization of International Conferences on Coordination Chemistry.

President BÉNARD had been given a mandate to call those interested, other than Members of the Division Committee, together. This meeting would take

place in Cortina on 5th July. Conclusions will be reached after the XIIth International Conference on Coordination Chemistry in Melbourne in August.

#### **4. Composition of Division Committee**

Prof. BÉNARD was retiring from the Presidency. Prof. GLEMSER was proposed as President and Prof. GUTMANN as Vice-President for the period 1969-1973.

Three Titular Members were leaving the Division Committee: Profs. BÉNARD and SARTORI and Dr. WICHERS. The following new Members were proposed: Prof. N. N. GREENWOOD (UK), Chairman of Commission II.1; Dr. W. S. HORTON (USA), Chairman of Commission II.3; and Prof. L. MALATESTA (Italy).

Prof. BÉNARD extended the hearty thanks of the Division Committee to Prof. SARTORI and Dr. WICHERS for their work in the Inorganic Chemistry Division.

## COMMISSION II.1: ATOMIC WEIGHTS

### I. Introduction

The Commission met in Cortina d'Ampezzo on 2nd and 3rd July, with Titular Members WICHERS, GUÉRON, FUJIWARA, GREENWOOD, PEISER, THODE, WAPSTRA, and Associate Members CAMERON and ROTH in attendance. The meetings had been preceded by a number of informal conferences between Members of the Commission and other interested persons and by an extensive exchange of correspondence.

In the administrative portion of the meetings at Cortina, Dr. CAMERON (USA) and Prof. ROTH (France) were elected to Titular Membership to succeed Dr. GUÉRON, whose term expired, and Dr. WICHERS, who retired on completion of 2 years of his current term of 4 years. Prof. GREENWOOD was elected Chairman of the Commission to succeed Dr. WICHERS, and Mr. PEISER was elected Secretary to succeed Dr. GUÉRON.

The current report is the first since that issued in 1961 to include any general discussion of problems in the Commission's area of responsibility. In that year, the provisional decision of 1959 was confirmed—to change the scale of atomic weights to one based on the number 12 as the assigned relative atomic mass of the carbon isotope 12. The provisional character of the earlier actions hinged on a similar action by the International Union of Pure and Applied Physics, which was taken by that Union in 1960. The change of scale necessitated a complete recalculation of the Table of Atomic Weights. This necessity, in turn, prompted a comprehensive review of the many changes in atomic weight values that had been adopted since the last previous general revision in 1925.

The biennial reports of the Commission since 1961 have dealt only with a limited number of recommended changes in the Table. The relatively small amount of relevant experimental work published in the interval has left unanswered questions about the reliability of many atomic weight values. Pending the appearance of such new measurements, the Commission has attempted this year to assess the uncertainties of all values in the Table, so that users may be able to distinguish their relative magnitudes. The discussion of this new treatment, together with matters of related interest, constitutes a large part of the following text of the 1969 Report.

### 2. Historical Perspective

The fundamental concept of Dalton's atomic theory was that matter can be differentiated into a limited number of elemental species, each composed of identical and immutable particles characterized, among other properties, by unique mass. The identification of all the elemental species and the determination of their characteristic atomic masses (relative to a common standard) constituted two of the great tasks of chemistry throughout the nineteenth century and the early decades of the twentieth. Realization of the importance (to chemical communication) of agreement on atomic weights led first to the formation of national committees in several of the leading countries and a little later to the establishment of the present Commission, which has dealt with the subject ever since through the publication of tables of recommended values. These tables have received world-wide acceptance.

The discovery of natural radioactivity, of the existence of stable isotopic variants of elements, and of the transmutability of elements, have made it necessary to qualify many of the concepts on which the work of the Commission was historically based. Geological events, laboratory handling, and



industrial processes can change isotopic composition. The time has long passed when such changes could always be ignored when compared with experimental uncertainties in atomic weight values. Moreover, a rapid increase in human handling of extraterrestrial materials can be expected. In keeping with these developments, the Commission has modified continually its modes of operation and reporting. Because its biennial reports now serve widely diversified interests in the field of chemistry, it is deemed desirable in the current Report to include a brief retrospective view of their evolution since the Commission was first created, near the beginning of the present century, and to foreshadow some of the problems which face the Commission, and indeed, every student of chemistry in the years ahead.

### 3. Explanation of Terms

*Atomic Weight.* From time to time, it has been suggested that the designation *atomic weight* should be replaced by *atomic mass* on the grounds that the latter is the property of primary interest and that this property does not have the dimensions of a force. It has also been proposed that the modifier *relative* be added. In 1961 the Commission, in fact, recommended the adoption of both changes. The addition of *relative* was approved, but not the change to *mass*, by higher administrative bodies in IUPAC.

This question has been reviewed at the current meeting of the Commission with the conclusion—agreed to with misgivings by some Members—that the traditional designation *atomic weight* should be retained. The reasons for this decision are as follows:

(a) The term *atomic weight* has a traditional meaning that is well understood by those who use the Table. It is unambiguous when qualified by the language of this explanatory statement.

(b) The term *atomic mass* (whether absolute or relative) should be reserved for nuclides as distinguished from elements. A table of *Atomic Masses* is published with the encouragement of the Commission on Atomic Masses and Related Constants (IUPAP). To avoid confusion, the term *atomic mass* should be reserved for that use. To use the same term for the quantity that is of interest in most chemical usage, it would have to be modified to indicate (i) that the number represents for most elements the average mass of a mixture of nuclides, and (ii) that this mixture is a naturally occurring one. Even if these precautions were taken, confusion would not be eliminated and errors would result because of the very similarity of many numbers expressing atomic weights and atomic masses of elemental and nuclidic species, respectively.

(c) The modifier *relative* is essentially redundant. The concept of relativity is implicit in the chemist's understanding of the term.

(d) Change to *atomic mass* would not remove the basic objection that *atomic weight* can mislead students on the *dimensions* of the numbers in the tables. On the contrary, the danger that students may assign units of mass in error is greater if we speak of atomic mass than that they assign units of force if we speak of atomic weight. In fact, the values should be regarded as dimensionless. To convert to the *Système International*, the values given must be multiplied by one-twelfth of the mass of a  $^{12}\text{C}$  atom; i.e., by the factor  $1.660\,432 \times 10^{-27}$  kg (or revisions of this value).

(e) Once we accept the *atomic weight* value as pure ratio, the equality with *atomic mass* (in the chemist's sense) depends only on the linearity of the relations between inertial mass, gravitational mass, and weight force. The requirement that atomic weight comparisons are deemed as made in the same gravitational field is self-evident.

*Isotope.* The etymological derivation of this word connotes plural forms. However, the term is often mistakenly used to refer not to one of two or more forms of an element, but to an inherently singular form. Correct usage is to say, for example, *sodium has no known natural isotope*; incorrect usage, *sodium exists in nature as a single isotope*. The latter situation can be described as *anisotropic*, i.e., *without isotopes*. Alternative language would be to say that sodium (in nature) is mononuclidic and that an element that exists in several isotopic forms is polynuclidic.

*Nuclide.* This is a useful word, proposed by T. P. KOHMAN, to designate an atomic species composed of a unique number of protons together with a unique number of neutrons. It does not seem to have gained uniform acceptance, because of a supposed likely confusion with nucleus. It is used occasionally in this Report, usually in the adjectival form, nuclidic, as in mononuclidic or polynuclidic.

*Differences in Atomic Weight Values.* A significant difference between atomic weight values for two experimental determinations or applicable to two isotopic compositions is a difference greater than one unit in the last digit of the atomic weight value for a specified element.

Discrepancies and uncertainties in atomic weight values are best stated in atomic weight units, rather than as fractions, percentages, ppm, etc.

*‘Normal’ Material.* A normal material is one that contains as a major constituent a specified element with an atomic weight value that does not display a significant difference from the accepted value of that atomic weight because of:

- (a) its radiogenic source;
- (b) its extraterrestrial origin;
- (c) artificial alteration;
- (d) mutation; or
- (e) a rare geological occurrence in small quantity.

#### 4. Variations in Isotopic Composition

The discovery that most chemical elements exist in nature as isotopic mixtures, many of which are known to vary in composition, makes it necessary to modify the historical concept of atomic weights as constants of nature. Even though isotopes have not been observed in nature for some elements (currently 21 in number), it appears more logical to consider that isotopic mixtures represent the normal rather than the exceptional state of an element. The Commission considers that this attitude will promote an awareness that uncertainties in the values given in the International Table are no longer, as in earlier times, to be regarded as resulting only from errors in the measurement of the value, but that they also arise from natural variations in isotopic composition.

Carried to its logical extreme, this view would mean that an atomic weight characterizes only a particular specimen of the element in question. Fortunately, this potentially extreme situation will seldom be encountered and for most of the purposes of chemistry, atomic weights can still be regarded as constants of nature, within limits. The Commission regards one of its functions to be to define these limits numerically, wherever possible, and in

general to append to the information given in its Report, all pertinent caveats. In assessing variations in isotopic composition, the Commission will continue to disregard other than *normal* materials.

To arrive at the recommended value for an atomic weight, the Commission will use weighting procedures so that the value will be optimized for materials in world science, chemical technology, and trade, rather than represent an estimated geochemical average.

### 5. Systematic Treatment of Uncertainties

Uncertainties in values for atomic weights arise not only from experimental errors of measurement, random or systematic, but also from variations in the relative abundances of the isotopes in the (isotopic) mixtures that constitute most of the elements as they exist in nature. In recent years, the Commission has appended to the Table information about the magnitudes, when known, of uncertainties arising from these two separate sources. However, the Commission now considers that the matter of primary interest to most users of the Table is the magnitude of the total uncertainty rather than its source or sources. Consequently, in the current Report, the publication of the separate supplementary tables of uncertainties resulting from experimental errors and variable isotopic compositions has been discontinued and the total estimated uncertainty indicated in the following manner. When adequate information is contained in the source publication, the estimated uncertainty is taken as three times the standard deviation of the experimental measurements from which the atomic weight value is calculated, plus the maximum difference between the stated value and that for any reliably observed normal material (see Section 3 for exclusions). Because this treatment makes no provision for systematic errors of measurement, such errors can be dealt with only by careful scrutiny of the source information for evidence that they (unless actually determined) are negligible in comparison with the random errors. Fortunately, modern procedures applicable to the determination of atomic weights and a general awareness among practitioners of the necessity for avoiding significant systematic errors facilitate the Commission's task of exercising critical judgments of the reliability of source information. No doubt some of these judgments will be found to be wrong, as time goes on.

It has been well known to the Commission, and to many users of the Table as well, that the tabulated values have had a considerable range of reliability. To aid users in recognizing the relative reliability of a particular value, the Commission has introduced a means of discrimination designed to supplement the information supplied by the number of significant figures used for each value. If the last digit of decimals is printed in the normal-type size, the estimated total uncertainty of the value does not exceed  $\pm 1$  in that digit. If this uncertainty is between  $\pm 1$  and  $\pm 3$  units, the last digit is printed in small-sized type. If the calculated uncertainty should be larger than  $\pm 3$  in a terminal digit, the number of digits will be decreased by one.

### 6. Changes of Values Based on New Experimental Work

*Lithium.* The atomic weight of lithium recommended in the 1961 revision of the Table of Atomic Weights was 6.939 and was based upon recalculation of the chemical ratios determined by RICHARDS and WILLARD<sup>1</sup>. There were no calibrated determinations of the isotopic composition at that time. Recently, some mass spectrometric measurements were reported which showed that lithium was variable in isotopic composition in nature. SVEC and ANDERSON<sup>2</sup> have reported measurements of the absolute abundance of the lithium isotopes



in natural sources. From their work the atomic weight of lithium is taken as 6.94,\* (with a limit of  $\pm 0.002$  to account for the variability with origin and to some extent with variability introduced in purification procedures).

**Rubidium.** In a recent investigation of the isotopes of rubidium, CATANZARO, MURPHY, GARNER and SHIELDS<sup>3</sup> find the abundances of <sup>85</sup>Rb and <sup>87</sup>Rb to be  $72.1654 \pm 0.0132$  and  $27.8346 \pm 0.0132$  atom percent, respectively. The formal treatment of random errors and the evidence for the exclusion of significant systematic errors justifies recommending 85.467<sup>8</sup> as the value for the atomic weight. The atomic masses of the rubidium isotopes were taken from the current atomic mass table of WAPSTRA and GOVE<sup>4</sup>. The new value agrees with the formerly listed value, 85.47, within its more limited precision. The earlier value was based on the comparison of rubidium chloride with silver and of rubidium bromide with silver and silver bromide by ARCHIBALD, HOOLEY and PHILLIPS, confirmed by mass spectrometric measurements by NIER (see 1961 Report).

**Lead.** The isotopic composition of *common* lead is variable because different ore bodies have received different contributions of radiogenic lead from uranium and thorium decay. In the revision of the Table of Atomic Weights in 1961, the value of 207.19 was chosen as representing lead likely to be encountered in normal laboratory work.

The isotopic compositions of lead ores from all over the world have been tabulated in three groups in an article by BROWN<sup>5</sup>:

World-wide, Paleozoic to Recent

207.220 to 207.271

World-wide, Precambrian

207.213 to 207.293

Mississippi Valley Type Deposits

207.198 to 207.207

The six *common* leads for which CATANZARO *et al.*<sup>6</sup> have published atomic weights range from 207.184 to 207.241.

In view of the rather wide range shown in these publications, the Commission recommends that the value in the Table be revised to 207.2. If a more precise atomic weight of a given specimen of lead is needed, the isotopic composition of the material must be ascertained to assist in this determination.

## 7. Other Recommended Changes in the Table

The newly adopted systematic treatment of uncertainties resulted in a large number of changes in the values published in the 1967 Table. In fact, only 27 of the 83 values in that Table remain unchanged in the new Table. The changes fall into groups as follows.

**Decreased Apparent Precision.** Six values appear with a smaller number of significant figures than in 1967. These elements are hydrogen, boron, carbon, sulfur, samarium, and lead (discussed more fully in the previous Section). For the first four of these, the respective uncertainties, due to natural variations in isotopic abundance, were formerly stated in a supplementary table, now discontinued. For samarium, the change resulted from a new evaluation of work previously published (see 1961 Report).

There are 28 additional elements for which the review of probable uncertainties resulted in changing the last digit from normal to small type. For five of these: oxygen, neon, silicon, iron, and copper, the uncertainties were previously stated in supplementary tables. For the remaining 23, the use of small type for the last digit provides a convenient classification of elements

\* 1 = one

whose atomic weight values are considered to have an intermediate degree of reliability between that implied by the use of a given number of significant figures as opposed to the use of one fewer digit. Apart from the warning to users of the Table suggested by this classification, it is to be hoped that the need for new determinations for several elements will thereby be made apparent. The 23 elements in the group are: argon, potassium, titanium, nickel, zinc, germanium, selenium, molybdenum, ruthenium, tin, antimony, tellurium, barium, neodymium, gadolinium, dysprosium, erbium, ytterbium, hafnium, wolfram (tungsten), platinum, mercury, and thallium.

In this connection, attention should also be drawn to four elements whose atomic weights are now stated to only a single decimal place. They are palladium, samarium, osmium, and rhenium.

*Increased Precision.* The values for the following 20 elements are given in the 1969 Table with a larger number of significant figures than in the 1967 Table: helium, beryllium, scandium, vanadium, rubidium, yttrium, niobium, rhodium, caesium, lanthanum, praseodymium, terbium, holmium, thulium, tantalum, iridium, gold, bismuth, thorium, and uranium.

Of the foregoing, 13 are mononuclidic elements whose atomic weights, in the absence of known natural isotopes, can be considered identical with the atomic masses of the only known naturally occurring nuclides of the respective elements. These atomic masses can be determined much more precisely than can the atomic weights of polynuclidic elements. In the 1969 Table these values are uniformly given to four decimal places, except for beryllium for which a comparable precision requires that five decimal places be used.

For the remaining elements, except helium, rubidium, and uranium, the added digit is in small type. Of these exceptions, the value for rubidium shows two additional digits; the second is in small type.

## 8. New Listings

In recent years, the International Table has not included values for the atomic weights of radioactive elements, except thorium and uranium, on the ground that they were seldom encountered in laboratory practice. Because this situation is changing, atomic weight values appear in the 1969 Table for four other radioactive elements that are now technologically important in the form of single nuclidic species. They are technetium-99, radium-226, protactinium-231, and neptunium-237. This is considered to be a desirable departure from the previous general rule of omitting atomic weight values for radioactive elements.

## 9. Discussion of Footnotes to the Table of Atomic Weights

Many of the values in the Table are referenced to one or more of seven footnotes that provide information that is of special interest or significance. These footnotes should invariably be included when the Table is reprinted in text or reference books or in related publications.

*Footnote a:* 'Mononuclidic element'. This footnote implies great accuracy of atomic weight value, as has been discussed in this and previous Commission reports (see, for example, that for 1961) (see also comment in paragraph 2 of Section II).

*Footnote b:* 'Element with one predominant isotope (about 99-100% abundance)'. The implication of this footnote is that errors or variations in relative abundance measurements will have a rather small effect on the atomic weight values.

*Footnote c:* 'Element for which the atomic weight is based on calibrated measurements'. This footnote implies confidence in reliability of atomic weight value through careful physical measurements based on comparisons with synthetic mixtures of almost pure isotopes. To this date, the only atomic weight values that in the Commission's judgment qualify for this annotation have been derived from mass spectrometry.

*Footnote d:* 'Element for which variation in isotopic abundance in terrestrial samples limits the precision of the atomic weight given'. Whereas at the present time only a few atomic weights of lighter elements (and those of copper and lead) are qualified by this footnote, one must expect an ever increasing number of atomic weight values to require this annotation. This trend is a natural consequence of greater precision of experimental determination and of progressively increasing information on variable isotopic composition of normal materials. It is most difficult to assess the reliability of many atomic weight values in the absence of good information on isotopic variability. The Commission has been conscious of the possible systematic errors that may be involved. Germanium is an example of such an element, which for this or other reasons is likely to need an upward adjustment when better data become available. It is, however, a well established principle of the Commission to revise values only on the basis of published work that in the judgment of the Commission advances significantly the confidence to be placed in the value.

*Footnote e:* 'Element for which users are cautioned against the possibility of large variations in atomic weight due to inadvertent or undisclosed artificial isotopic separation in commercially available materials'. The seriousness of the hazard must be stressed for users of atomic weight values qualified by footnote e. The atomic weight values given in the Table are neither adjusted nor is their implied accuracy limited to include significant human interference in isotopic abundance. Suppliers of an otherwise well characterized chemical containing as a major constituent one of the elements so annotated should consider the desirability of either supplying the relevant atomic weight value or certifying the virgin source of the raw material plus a statement of the extent to which subsequent processing is expected to have changed the isotopic abundance. In this Report this footnote applies only to lithium, boron, and uranium. It can be foreseen, however, that advancing technology will gradually introduce such complications for other elements. Time is not far off, for example, when fission products will be introduced into normal trade. The Commission clearly must keep this situation under careful and continuing review.

*Footnote f:* 'Most commonly available long-lived isotope; see *Table of Selected Radioactive Isotopes*'. The situation described by footnote f is similar in effect to that covered by footnote e. The user is warned that materials containing this element may display an unusual atomic weight value. Whereas for footnote e, such material arose through isotopic separation, footnote f concerns materials with differing histories of radioactive, fission, or other nuclear processes. Footnote f concerns developments that will become more critical with continuing advance of nuclear technology.

*Footnote g:* 'In some geological specimens this element has a highly anomalous isotopic composition, corresponding to an atomic weight significantly different from that given'. The significance of this footnote is clear, and its application to lead and strontium (from rubidium-containing geological sources) is not difficult to justify. The Commission must attempt to state the atomic weight values so that they are as precise as possible. At the same



time, they must be sufficiently imprecise so that all normal specimens fall within the implied tolerance range. In other words, large quantities of available materials should not lie outside the tolerance range. The difficult judgment has to be made when only a small fraction of normal material falls outside the tolerance range. The Commission has decided in such cases not to discard useful accuracy applicable to the great majority of practical conditions, but to exclude from the definition of *normal*, geological oddities.

### **10. Selected Radioactive Isotopes**

In addition to its primary purpose of providing internationally recommended values for atomic weights, the International Table is also useful as a convenient listing of the names, symbols, and atomic numbers of all the chemical elements. For this reason, it is included in many chemical textbooks and handbooks. In the International Table, atomic weights are given only for those radioactive elements, whether natural or artificial, that are important in chemical technology and for which such an atomic weight is, in practice at least, unique. The radioactive elements are also listed in a supplemental table that provides current information on the half-lives of selected isotopes, together with the modes of disintegration of these isotopes. The supplemental table is updated in each biennial report. In the 1969 Report, the Commission has introduced, on an experimental basis, one innovation: where more than one isotope of a radioactive element is held to be of technical importance, each has been listed.

For the updating of this table, the Commission is particularly grateful to colleagues of Dr. J. SPAEPEN at the Geel Laboratories of Euratom and to A. SPERNOL in particular who carried out the literature compilation which can be obtained by request from the Commission Secretary.

The values of the half-lives are in general uncertain to  $\pm 1$  in the last given digit. If this last digit is set in small type, the estimated uncertainty is  $\pm 3$  in this digit.

### **11. Atomic Masses of Selected Isotopes**

Certain of the chemical elements, as obtained from commercial sources, are likely to have isotopic compositions that differ markedly from those in natural sources. Notable examples are lithium, boron, and uranium. If either the isotopic composition or the atomic weight is a matter of concern, users of these elements should measure or otherwise ascertain the isotopic composition of the material at hand. Atomic weights can be calculated by using the supplemental table of atomic masses of the pertinent isotopes. The relevant figures are taken from WAPSTRA, KURZECK and ANISIMOFF<sup>7</sup> for heavy nuclides, and from WAPSTRA and GOVE<sup>4</sup> for other atomic masses.

By the data from WAPSTRA *et al.*<sup>4,7</sup> and the error analyses of these authors there is in most cases a little additional accuracy which is being disregarded in the tables in this Report. Users requiring the greatest available accuracy in atomic mass values should therefore consult the referenced papers.

When these values are used as intended, that is for the atomic weights of elements, there exists the possibility of small systematic error from undiscovered stable isotopes present in very small amounts.

### **12. New Techniques for Atomic Weight Determinations**

The Commission has set itself the task to keep currently informed on a number of new physical and physicochemical techniques that may lead to significant atomic weight determinations.

At the current session, it heard a discussion by one of its members, Dr. FUJIWARA, on his atomic mass determination of  $^{40}\text{Ar}$  by ion cyclotron resonance. This work is at least close to being limited by uncertainties in the accuracy of the available values of fundamental physical constants such as Avogadro's Number, the magnetic dipole moment of the proton, *etc.* The atomic mass value could thus be used alternatively to help refine the fundamental constants.

Even for the evaluation of isotopic abundances resonance methods may become applicable. The Commission therefore looks forward to active future developments in atomic weight evaluations by possible significant challenges from a diversity of methods.

### 13. Erratum in Table of Atomic Weights 1967

In the 1967 Table (*Comptes Rendus XXIV Conference*) the uncertainty relating to the value for copper was erroneously entered in the list of experimental uncertainties (footnote b). It should have been entered among the uncertainties governed by variations in natural abundances (footnote a). The reference in the table at the copper value was correctly given to footnote a.

### 14. Table of Atomic Weights 1969

BASED ON THE ASSIGNED RELATIVE ATOMIC MASS OF  $^{12}\text{C} = 12$

The following values apply to elements as they exist in materials of terrestrial origin and to certain artificial elements. When used with due regard to the footnotes, they are considered reliable to  $\pm 1$  in the last digit, or  $\pm 3$  if that digit is in small type.

Alphabetical Order in English

Name	Symbol	Atomic Number	Atomic Weight	Name	Symbol	Atomic Number	Atomic Weight
Actinium	Ac	89	..	Copper	Cu	29	63.546 <sup>c,d</sup>
Aluminium	Al	13	26.9815 <sup>a</sup>	Curium	Cm	96	..
Americium	Am	95	..	Dysprosium	Dy	66	162.5 <sub>0</sub>
Antimony	Sb	51	121.7 <sub>5</sub>	Einsteinium	Es	99	..
Argon	Ar	18	39.948 <sup>b,c,d,g</sup>	Erbium	Er	68	167.2 <sub>6</sub>
Arsenic	As	33	74.9216 <sup>a</sup>	Europium	Eu	63	151.96
Astatine	At	85	..	Fermium	Fm	100	..
Barium	Ba	56	137.3 <sub>4</sub>	Fluorine	F	9	18.9984 <sup>a</sup>
Berkelium	Bk	97	..	Francium	Fr	87	..
Beryllium	Be	4	9.01218 <sup>a</sup>	Gadolinium	Gd	64	157.2 <sub>5</sub>
Bismuth	Bi	83	208.9806 <sup>a</sup>	Gallium	Ga	31	69.72
Boron	B	5	10.81 <sup>c,d,e</sup>	Germanium	Ge	32	72.5 <sub>9</sub>
Bromine	Br	35	79.904 <sup>c</sup>	Gold	Au	79	196.9665 <sup>a</sup>
Cadmium	Cd	48	112.40	Hafnium	Hf	72	178.4 <sub>9</sub>
Calcium	Ca	20	40.08	Helium	He	2	4.00260 <sup>b,c</sup>
Californium	Cf	98	..	Holmium	Ho	67	164.9303 <sup>a</sup>
Carbon	C	6	12.011 <sup>b,d</sup>	Hydrogen	H	1	1.008 <sub>0</sub> <sup>b,d</sup>
Cerium	Ce	58	140.12	Indium	In	49	114.82
Cesium	Cs	55	132.9055 <sup>a</sup>	Iodine	I	53	126.9045 <sup>a</sup>
Chlorine	Cl	17	35.453 <sup>c</sup>	Iridium	Ir	77	192.2 <sub>2</sub>
Chromium	Cr	24	51.996 <sup>c</sup>	Iron	Fe	26	55.84 <sub>7</sub>
Cobalt	Co	27	58.9332 <sup>a</sup>	Krypton	Kr	36	83.80

Name	Symbol	Atomic Number	Atomic Weight	Name	Symbol	Atomic Number	Atomic Weight
Lanthanum	La	57	138.905 <sub>5</sub> <sup>b</sup>	Rhenium	Re	75	186.2
Lawrencium	Lr	103	..	Rhodium	Rh	45	102.9055 <sup>a</sup>
Lead	Pb	82	207.2 <sup>d,g</sup>	Rubidium	Rb	37	85.467 <sub>8</sub> <sup>c</sup>
Lithium	Li	3	6.941 <sup>c,d,e</sup>	Ruthenium	Ru	44	101.0 <sub>7</sub>
Lutetium	Lu	71	174.97	Samarium	Sm	62	150.4
Magnesium	Mg	12	24.305 <sup>c</sup>	Scandium	Sc	21	44.9559 <sup>a</sup>
Manganese	Mn	25	54.9380 <sup>a</sup>	Selenium	Se	34	78.9 <sub>6</sub>
Mendelevium	Md	101	..	Silicon	Si	14	28.08 <sub>6</sub> <sup>d</sup>
Mercury	Hg	80	200.5 <sub>9</sub>	Silver	Ag	47	107.868 <sup>c</sup>
Molybdenum	Mo	42	95.9 <sub>4</sub>	Sodium	Na	11	22.9898 <sup>a</sup>
Neodymium	Nd	60	144.2 <sub>4</sub>	Strontium	Sr	38	87.62 <sup>g</sup>
Neon	Ne	10	20.17 <sub>9</sub> <sup>c</sup>	Sulfur	S	16	32.06 <sup>d</sup>
Neptunium	Np	93	237.0482 <sup>b,f</sup>	Tantalum	Ta	73	180.947 <sub>9</sub> <sup>b</sup>
Nickel	Ni	28	58.7 <sub>1</sub>	Technetium	Tc	43	98.9062 <sup>f</sup>
Niobium	Nb	41	92.9064 <sup>a</sup>	Tellurium	Te	52	127.6 <sub>0</sub>
Nitrogen	N	7	14.0067 <sup>b,c</sup>	Terbium	Tb	65	158.9254 <sup>a</sup>
Nobelium	No	102	..	Thallium	Tl	81	204.3 <sub>7</sub>
Osmium	Os	76	190.2	Thorium	Th	90	232.0381 <sup>a,f</sup>
Oxygen	O	8	15.999 <sub>4</sub> <sup>b,c,d</sup>	Thulium	Tm	69	168.9342 <sup>a</sup>
Palladium	Pd	46	106.4	Tin	Sn	50	118.6 <sub>9</sub>
Phosphorus	P	15	30.9738 <sup>a</sup>	Titanium	Ti	22	47.9 <sub>0</sub>
Platinum	Pt	78	195.0 <sub>9</sub>	Tungsten	W	74	183.8 <sub>5</sub>
Plutonium	Pu	94	..	Uranium	U	92	238.029 <sup>b,c,e</sup>
Polonium	Po	84	..	Vanadium	V	23	50.941 <sub>4</sub> <sup>b,c</sup>
Potassium	K	19	39.10 <sub>2</sub>	Wolfram	W	74	183.8 <sub>5</sub>
Praseodymium	Pr	59	140.9077 <sup>a</sup>	Xenon	Xe	54	131.30
Promethium	Pm	61	..	Ytterbium	Yb	70	173.0 <sub>4</sub>
Protactinium	Pa	91	231.0359 <sup>a,f</sup>	Yttrium	Y	39	88.9059 <sup>a</sup>
Radium	Ra	88	226.0254 <sup>a,f,g</sup>	Zinc	Zn	30	65.3 <sub>7</sub>
Radon	Rn	86	..	Zirconium	Zr	40	91.22

<sup>a</sup> Mononuclidic element.

<sup>b</sup> Element with one predominant isotope (about 99-100% abundance).

<sup>c</sup> Element for which the atomic weight is based on calibrated measurements.

<sup>d</sup> Element for which variation in isotopic abundance in terrestrial samples limits the precision of the atomic weight given.

<sup>e</sup> Element for which users are cautioned against the possibility of large variations in atomic weight due to inadvertent or undisclosed artificial isotopic separation in commercially available materials.

<sup>f</sup> Most commonly available long-lived isotope (see *Table of Selected Radioactive Isotopes*).

<sup>g</sup> In some geological specimens this element has a highly anomalous isotopic composition, corresponding to an atomic weight significantly different from that given.



## 15. Table of Atomic Weights 1969

BASED ON THE ASSIGNED RELATIVE ATOMIC MASS OF  $^{12}\text{C} = 12$

The following values apply to elements as they exist in materials of terrestrial origin and to certain artificial elements. When used with due regard to the footnotes, they are considered reliable to  $\pm 1$  in the last digit, or  $\pm 3$  if that digit is in small type.

### Order of Atomic Number

Atomic Number	Name	Symbol	Atomic Weight	Atomic Number	Name	Symbol	Atomic Weight
1	Hydrogen	H	1.008 <sup>o,b,d</sup>	42	Molybdenum	Mo	95.9 <sub>4</sub>
2	Helium	He	4.00260 <sup>b,c</sup>	43	Technetium	Tc	98.9062 <sup>f</sup>
3	Lithium	Li	6.94 <sub>1</sub> <sup>c,d,e</sup>	44	Ruthenium	Ru	101.0 <sub>7</sub>
4	Beryllium	Be	9.01218 <sup>a</sup>	45	Rhodium	Rh	102.9055 <sup>a</sup>
5	Boron	B	10.81 <sup>c,d,e</sup>	46	Palladium	Pd	106.4
6	Carbon	C	12.011 <sup>b,d</sup>	47	Silver	Ag	107.868 <sup>c</sup>
7	Nitrogen	N	14.0067 <sup>b,c</sup>	48	Cadmium	Cd	112.40
8	Oxygen	O	15.999 <sub>4</sub> <sup>b,c,d</sup>	49	Indium	In	114.82
9	Fluorine	F	18.9984 <sup>a</sup>	50	Tin	Sn	118.6 <sub>9</sub>
10	Neon	Ne	20.17 <sub>9</sub> <sup>c</sup>	51	Antimony	Sb	121.7 <sub>5</sub>
11	Sodium	Na	22.9898 <sup>a</sup>	52	Tellurium	Te	127.6 <sub>0</sub>
12	Magnesium	Mg	24.305 <sup>c</sup>	53	Iodine	I	126.9045 <sup>a</sup>
13	Aluminium	Al	26.9815 <sup>a</sup>	54	Xenon	Xe	131.30
14	Silicon	Si	28.08 <sup>6d</sup>	55	Cesium	Cs	132.9055 <sup>a</sup>
15	Phosphorus	P	30.9738 <sup>a</sup>	56	Barium	Ba	137.3 <sub>4</sub>
16	Sulfur	S	32.06 <sup>d</sup>	57	Lanthanum	La	138.905 <sub>5</sub> <sup>b</sup>
17	Chlorine	Cl	35.453 <sup>c</sup>	58	Cerium	Ce	140.12
18	Argon	Ar	39.94 <sub>8</sub> <sup>b,c,d,g</sup>	59	Praseodymium	Pr	140.9077 <sup>a</sup>
19	Potassium	K	39.10 <sub>2</sub>	60	Neodymium	Nd	144.2 <sub>4</sub>
20	Calcium	Ca	40.08	61	Promethium	Pm	..
21	Scandium	Sc	44.9559 <sup>a</sup>	62	Samarium	Sm	150.4
22	Titanium	Ti	47.9 <sub>0</sub>	63	Europium	Eu	151.96
23	Vanadium	V	50.941 <sub>4</sub> <sup>b,c</sup>	64	Gadolinium	Gd	157.2 <sub>5</sub>
24	Chromium	Cr	51.996 <sup>c</sup>	65	Terbium	Tb	158.9254 <sup>a</sup>
25	Manganese	Mn	54.9380 <sup>a</sup>	66	Dysprosium	Dy	162.5 <sub>0</sub>
26	Iron	Fe	55.84 <sub>7</sub>	67	Holmium	Ho	164.9303 <sup>a</sup>
27	Cobalt	Co	58.9332 <sup>a</sup>	68	Erbium	Er	167.2 <sub>6</sub>
28	Nickel	Ni	58.7 <sub>1</sub>	69	Thulium	Tm	168.9342 <sup>a</sup>
29	Copper	Cu	63.54 <sub>6</sub> <sup>c,d</sup>	70	Ytterbium	Yb	173.0 <sub>4</sub>
30	Zinc	Zn	65.3 <sub>7</sub>	71	Lutetium	Lu	174.97
31	Gallium	Ga	69.72	72	Hafnium	Hf	178.4 <sub>9</sub>
32	Germanium	Ge	72.5 <sub>9</sub>	73	Tantalum	Ta	180.947 <sub>9</sub> <sup>b</sup>
33	Arsenic	As	74.9216 <sup>a</sup>	74	Wolfram (Tungsten)	W	183.8 <sub>5</sub>
34	Selenium	Se	78.9 <sub>6</sub>	75	Rhenium	Re	186.2
35	Bromine	Br	79.904 <sup>c</sup>	76	Osmium	Os	190.2
36	Krypton	Kr	83.80	77	Iridium	Ir	192.2 <sub>2</sub>
37	Rubidium	Rb	85.467 <sub>8</sub> <sup>c</sup>	78	Platinum	Pt	195.0 <sub>9</sub>
38	Strontium	Sr	87.62 <sup>g</sup>	79	Gold	Au	196.9665 <sup>a</sup>
39	Yttrium	Y	88.9059 <sup>a</sup>	80	Mercury	Hg	200.5 <sub>9</sub>
40	Zirconium	Zr	91.22	81	Thallium	Tl	204.3 <sub>7</sub>
41	Niobium	Nb	92.9064 <sup>a</sup>	82	Lead	Pb	207.2 <sup>d,g</sup>

Atomic Number	Name	Symbol	Atomic Weight	Atomic Number	Name	Symbol	Atomic Weight
83	Bismuth	Bi	208.9806 <sup>a</sup>	94	Plutonium	Pu	..
84	Polonium	Po	..	95	Americium	Am	..
85	Astatine	At	..	96	Curium	Cm	..
86	Radon	Rn	..	97	Berkelium	Bk	..
87	Francium	Fr	..	98	Californium	Cf	..
88	Radium	Ra	226.0254 <sup>a, f, g</sup>	99	Einsteinium	Es	..
89	Actinium	Ac	..	100	Fermium	Fm	..
90	Thorium	Th	232.0381 <sup>a, f</sup>	101	Mendelevium	Md	..
91	Protactinium	Pa	231.0359 <sup>a, f</sup>	102	Nobelium	No	..
92	Uranium	U	238.029 <sup>b, c, e</sup>	103	Lawrencium	Lr	..
93	Neptunium	Np	237.0482 <sup>b, f</sup>				

<sup>a</sup> Mononuclidic element.

<sup>b</sup> Element with one predominant isotope (about 99-100% abundance).

<sup>c</sup> Element for which the atomic weight is based on calibrated measurements.

<sup>d</sup> Element for which variation in isotopic abundance in terrestrial samples limits the precision of the atomic weight given.

<sup>e</sup> Element for which users are cautioned against the possibility of large variations in atomic weight due to inadvertent or undisclosed artificial isotopic separation in commercially available materials.

<sup>f</sup> Most commonly available long-lived isotope (see *Table of Selected Radioactive Isotopes*).

<sup>g</sup> In some geological specimens this element has a highly anomalous isotopic composition, corresponding to an atomic weight significantly different from that given.

## 16. Table of Selected Radioactive Isotopes

### Order of Atomic Number

This table lists selected isotopes of the chemical elements, whether occurring in nature or known only through synthesis, that are commonly classed as radioactive. The listed isotopes include the one of longest known half-life and others of recognized interest. Decay modes with intensities below 0.01 % are not mentioned.

Atomic Number	Name	Symbol	Isotope	Half-Life*	Decay Mode**
43	Technetium	Tc	97	2.6·10 <sup>6</sup> y	EC
43	Technetium	Tc	99	2.14·10 <sup>5</sup> y	β <sup>-</sup>
61	Promethium	Pm	145	18.0 y	EC
61	Promethium	Pm	147	2.62 y	β <sup>-</sup>
84	Polonium	Po	209	1.0·10 <sup>2</sup> y	α, EC
84	Polonium	Po	210	138.4 d	α
85	Astatine	At	210	8.3 h	EC, α
86	Radon	Rn	222	3.82 d	α
87	Francium	Fr	223	22 m	β <sup>-</sup>
88	Radium	Ra	226	1.60·10 <sup>3</sup> y	α
89	Actinium	Ac	227	21.8 y	β <sup>-</sup> , α

Atomic Number	Name	Symbol	Isotope	Half-Life*	Decay Mode**
90	Thorium	Th	232	$1.41 \cdot 10^{10}$ y	$\alpha$
91	Protactinium	Pa	231	$3.26 \cdot 10^4$ y	$\alpha$
92	Uranium	U	233	$1.60 \cdot 10^5$ y	$\alpha$
92	Uranium	U	234	$2.47 \cdot 10^5$ y	$\alpha$
92	Uranium	U	235	$7.0 \cdot 10^8$ y	$\alpha$
92	Uranium	U	238	$4.5 \cdot 10^9$ y	$\alpha$
93	Neptunium	Np	237	$2.14 \cdot 10^6$ y	$\alpha$
94	Plutonium	Pu	238	87 y	$\alpha$
94	Plutonium	Pu	239	$24.3 \cdot 10^3$ y	$\alpha$
94	Plutonium	Pu	240	$6.6 \cdot 10^3$ y	$\alpha$
94	Plutonium	Pu	241	14.2 y	$\beta^-$
94	Plutonium	Pu	242	$3.86 \cdot 10^5$ y	$\alpha$
94	Plutonium	Pu	244	$8.2 \cdot 10^7$ y	$\alpha$ , s.f.
95	Americium	Am	241	43.5 y	$\alpha$
95	Americium	Am	243	$7.4 \cdot 10^3$ y	$\alpha$
96	Curium	Cm	242	164 d	$\alpha$
96	Curium	Cm	243	3.2 y	$\alpha$ , EC
96	Curium	Cm	244	18.1 y	$\alpha$
96	Curium	Cm	245	$8.3 \cdot 10^3$ y	$\alpha$
96	Curium	Cm	246	$4.7 \cdot 10^3$ y	$\alpha$ , s.f.
96	Curium	Cm	247	$1.6 \cdot 10^7$ y	$\alpha$
96	Curium	Cm	248	$3.5 \cdot 10^5$ y	$\alpha$ , s.f.
96	Curium	Cm	250	$1.1 \cdot 10^4$ y	s.f.
97	Berkelium	Bk	247	$1.4 \cdot 10^3$ y	$\alpha$
97	Berkelium	Bk	249	$3.1 \cdot 10^2$ d	$\beta^-$
98	Californium	Cf	251	900 y	$\alpha$
98	Californium	Cf	252	2.64 y	$\alpha$ , s.f.
98	Californium	Cf	254	60.5 d	s.f., $\alpha$
99	Einsteinium	Es	253	20 d	$\alpha$
99	Einsteinium	Es	254	$2.7 \cdot 10^2$ d	$\alpha$
100	Fermium	Fm	257	80 d	$\alpha$ , s.f.
101	Mendelevium	Md	257	3.0 h	EC, $\alpha$ , s.f.
101	Mendelevium	Md	258	54 d	EC, $\alpha$ , s.f.
102	Nobelium	No	255	18.5 s	$\alpha$ , EC
103	Lawrencium	Lr	256	3.5 s	$\alpha$

\* s—second; m—minute; h—hour; d—day; y—year.

\*\* EC—electron capture; s.f.—spontaneous fission.



**17. Table of Atomic Masses of Selected Isotopes**

Name	Symbol	Atomic Number	Mass Number	Atomic Mass
Hydrogen	H	1	1	1.00782
Deuterium	D	1	2	2.01410
Tritium	T	1	3	3.01605
Helium	He	2	3	3.01603
			4	4.00260
Lithium	Li	3	6	6.01512
			7	7.01600
Boron	B	5	10	10.0129
			11	11.0093
Carbon	C	6	12	12 exactly
			13	13.0034
			14	14.0032
Nitrogen	N	7	14	14.0031
			15	15.0001
Oxygen	O	8	16	15.9949
			17	16.9991
			18	17.9992
Sulfur	S	16	32	31.9721
			33	32.9715
			34	33.9679
			36	35.9671
Promethium	Pm	61	143	142.9110
			145	144.9128
			147	146.9152
Lead	Pb	82	204	203.9731
			206	205.9745
			207	206.9759
			208	207.9766
Uranium	U	92	233	233.0396
			234	234.0410
			235	235.0439
			236	236.0456
			238	238.0508
Plutonium	Pu	94	238	238.0496
			239	239.0522
			240	240.0538
			241	241.0569
			242	242.0588
			244	244.0642
Curium	Cm	96	242	242.0589
			244	244.0628
			246	246.0672
			247	247.0704
			248	248.0724

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## COMMISSION II.2: NOMENCLATURE OF INORGANIC CHEMISTRY

### 1. Meetings

The Commission met during the period 30th June-4th July. The following were present: JENSEN, REMY, GALLAIS, PRUE, ADAMS, CHATT, CHEESMAN, FERNELIUS, MALATESTA, ÖLANDER (Titular Members); REES (30th June) (Associate Member); BERTELLO, BUSCHBECK, LOENING, VEIBEL (4th July) (Observers).

### 2. Crystalline Phases of Variable Composition

Comments on the tentative rules were considered. At the request of the Chairman of Commission I.1, and subject to the concurrence of IUPAP, it was agreed to replace the symbol  $p^+$  to designate a positive hole by  $v^+$ , and the symbol  $\sim$  by  $\approx$ . A few other minor changes were also made. The revised rules were approved for publication as Section 9 in the new *Red Book*. The Working Party (minute 63/15) was thanked for its work and discharged.

### 3. $\pi$ -Complexes

From comments received on the tentative rules proposed for naming such compounds, it was clear that substantial revision was necessary. It was agreed that (a) a  $\sigma$ - $\pi$  system of nomenclature with electronic implications was undesirable, (b) the nomenclature should rather emphasize the geometrical relationship between ligands and central atom, and (c) the *hapto* nomenclature suggested by F. A. COTTON had much to commend it. The use of the symbol  $\eta$  for *hapto* was suggested. It was agreed to remove tentative rule 7.35 from the new *Red Book* and a Working Party (ADAMS, CHATT, FERNELIUS, LOENING) was appointed to draft a revised set of tentative rules. Some of the examples in 7.35 could be placed elsewhere in the revised Section 7 and a brief mention of  $\pi$ -complexes would still be necessary; Dr. FERNELIUS agreed to deal with this matter.

### 4. Revision of 1957 Rules (Red Book)

A final detailed review was made of the revised version of Sections 1, 2, 3, 5, 6, 7.7, and 8 of the 1957 Rules; this included consideration of the comments of the Chairman of the Hungarian Commission of Chemical Nomenclature. Most of the changes made dealt with inconsistencies between different sections which had arisen in the process of revision of the 1957 Rules, or were of a minor nature. The following changes and additions were also made:-

1.21—Insert as second sentence: The use of the collective names *pnictogen* (N, P, As, Sb and Bi) and *pnictides* is not approved (see also Item 10 of this Report).

2.15—Final paragraph to read: If the compound contains more than one electropositive or more than one electronegative constituent, the sequence within each class should be in alphabetical order of their symbols. Acids are treated as hydrogen salts, e.g.,  $H_2SO_4$  and  $H_2PtCl_6$ ; for the position of hydrogen see 6.323, cf. 6.2. To determine the position of complex ions only the symbol of the central atom is considered. For coordination compounds see 7.2.

2.161—Substitute for second paragraph: In the formulae of compounds containing two or more different atoms or groups attached to a single central atom, the symbol of the central atom shall be placed first, followed by the symbols of the remaining atoms or groups in alphabetical order, e.g.,  $PBrCl_2$ ,  $SbCl_2F$ ,  $PCl_3O$ ,  $P(NCO)_3O$ ,  $PO(OCN)_3$ .



2.17—To read: In intermetallic and similar compounds the constituents should be placed in alphabetical order of their symbols, with non-metals except Sb at the end in the order prescribed in 2.16. Deviations from this order may be allowed, *e.g.*, to emphasize ionic character as in  $\text{Na}_3\text{Bi}_5$ , or when compounds with analogous structures are compared, *e.g.*,  $\text{CuZn}$  and  $\text{CuCd}$ .

2.3—A short section on the names of hydrides (2.3) to be inserted before a section on trivial names (2.4).

*Index.* Section numbers to be given rather than page numbers.

All changes will be incorporated in the photocopy of the draft version of the new *Red Book* which will be circulated to members of the Commission as soon as possible (see Item 12 of this Report).

## 5. Coordination Compounds

In addition to several minor clarifications in Section 7 of the new *Red Book*, it was also agreed to add (a) a note to draw attention to the way in which the locant designator scheme gave different prefixes to enantiomers, (b) a list of abbreviations of common ligands (Dr. BUSCHBECK would supply a list of those used in Gmelin's *Handbuch*), (c) clarifications of the meaning of *complex expression*, the use of di- and bis-, *etc.*, and the use of enclosing marks. It was also agreed to replace by the word *represents* the symbol :, used as in the examples in the new Section 7.413 and subsequently, and that publication as an appendix of an article by McDONNELL and PASTERNAK (minute 66/9) was unnecessary. Dr. FERNELIUS agreed to prepare the final version of Section 7.

## 6. Iso- and Heteropolyanions

Subject to some redrafting of the final section dealing with *A General Nomenclature for Polyanions with Ring or Chain Structure* and a few other minor changes, with which Prof. JENSEN agreed to deal, the tentative rules were approved for publication as Section 4 in the new *Red Book*. Dr. FERNELIUS was asked to consider whether it was desirable to elaborate the conventions governing the use of the prefix *cyclo-*.

## 7. Boron Compounds

For inorganic compounds, draft rules based on the Hellerup discussions (minute 68/2) were presented by Prof. ADAMS and Dr. FERNELIUS. After detailed discussion and some amendments it was agreed that these should be published as tentative rules following the circulation to members of an amended draft for final approval.

It was agreed that a short section on boron compounds was desirable in the new *Red Book*. A draft of such a section prepared by Prof. JENSEN and based on the tentative rules published in 1966 was approved subject to editorial attention. This would be Section 11 of the new rules.

## 8. Names of Elements

It had become abundantly clear during the past year that nuclear physicists reporting the preparation of new elements were exceedingly strongly attached to the right of a discoverer to select a name, and reluctant to accept the Commission's principle that whilst early selection of a name was a matter of convenience it carried (Rule 1.12) no implication regarding priority of discovery. The Chairmen of Commissions II.1 and II.2 had discussed the matter, and suggested that in the present circumstances elements (including 104) should not be named until 5 years had elapsed after the initial announcement of their discovery. The period would it was hoped allow confirmation of the

initial discovery in another laboratory, and preferably in another country. The Commission still felt that absence of a systematic nomenclature was leading to needless controversy.

### **9. Section D of 'Nomenclature of Organic Chemistry' (Joint Publication of Inorganic Chemistry and Organic Chemistry Divisions)**

The Chairman reported on the meeting at Oberursel in May of Sub-Commission II.2.1. After discussion of the draft section on organic compounds of phosphorus, arsenic, antimony, and bismuth it was unanimously resolved that:

The Commission cannot accept a document in which Roman numerals are used as on pp. 35 and 36. If a symbol is required it must be different, *e.g.*, (v III) in place of (III), and defined. Its use as at present will produce untold confusion in well-established principles of inorganic nomenclature.

### **10. Collective Names for Groups of Elements**

In response to a letter received from Prof. E. F. WESTRUM, Jr., the Commission confirmed its disapproval of the use of the collective names *pnictogen* and *pnictides* (see Item 4 of this Report). With two abstentions the Commission agreed to recommend that if group names are needed they should be triels (B, Al, Ga, In and Tl), tetrels (C, Si, Ge, Sn and Pb) and pentels (N, P, As, Sb and Bi), with trielide, tetrelide and pentelide, respectively, for the binary compounds.

### **11. Nomenclature for Zeolites and Molecular Sieves (Natural and Synthetic)**

The Commission agreed to a proposal from Commission I.6 to establish a 4-membered Working Party with representatives from the two Commissions, the International Mineralogical Association and the International Union of Crystallography. The Commission appointed Prof. ÖLANDER as its representative. The Commission emphasized that eventual responsibility for IUPAC nomenclature rules for these compounds must rest with Commission II.2 alone.

### **12. Publication of Revised Rules (Red Book)**

Photocopies of the final draft will be circulated to all members as soon as possible. A Drafting Committee (ADAMS, CHATT, FERNELIUS, GALLAIS, LOENING, PRUE) was appointed to complete the final editing; it will also deal with the tentative rules for inorganic boron compounds (Item 7 of this Report) and for  $\pi$ -complexes (Item 3 of this Report).

### **13. Membership**

This was discussed in a meeting restricted to Titular Members. It was agreed that substantial changes would be appropriate after the new *Red Book* and Section D of *Nomenclature of Organic Chemistry* (Joint Publication of Inorganic Chemistry and Organic Chemistry Divisions) had been published.

## Commission II.3: High Temperatures and Refractories

### 1. Meeting

The Commission met on 4th July. The following were present: NOWOTNY, COLLONGUES, FLOOD, HORTON (Titular Members); CABANNES (Associate Member); HLAVÁČ, DE MARIA, RIECK (Observers).

### 2. Membership

The discussion of the future membership of the Commission was started by the remark from the Secretary that the Inorganic Chemistry Division will favourably consider an increase in the number of Titular Members in recognition of the activity already carried out and the future plans. The Commission unanimously decided the following proposal.

Because of the 8-year period Prof. NOWOTNY, Prof. FLOOD, Dr. BRIGHT, and Dr. WALKER have to step down from their present positions. It was proposed that Dr. HORTON will act as the new Chairman, and Prof. G. D. RIECK (Netherlands) agreed to act as Secretary for the period 1969-1973. It was proposed to name Prof. C. B. ALCOCK (UK), Prof. COLLONGUES, Prof. E. FITZER (USA), and either Prof. A. E. SHEINDLIN or Prof. L. V. GURVICH (USSR) as Titular Members for the same period. Furthermore, the following Associate Members were proposed: Prof. F. CABANNES, Prof. G. DE MARIA (Italy), Prof. J. HLAVÁČ (Czechoslovakia), Prof. T. MII (Japan), Prof. K. MOTZFELD (Norway), and Prof. NOWOTNY. It was also proposed to establish contacts through the National Societies for the delegation of National Representatives from the following countries: Australia, Belgium, Canada, India, Poland, Sweden, UK, and USA. The future Chairman will be encouraged to arrange these contacts.

### 3. Activities 1967-1969

Previous Commission meetings convened on the necessity to work on secondary temperature standards and vapor pressure standards for an international assessment. Through the initiative of Dr. HORTON, an appreciable amount of the planned work was organized within US National Bureau of Standards (NBS). Under Dr. HORTON's supervision Mr. S. J. SCHNEIDER acts as Coordinator of the Task Force on Secondary Temperature Standards, and Dr. R. C. PAULE, as Coordinator on the Task Force on Vapor Pressure Standard Reference Materials. According to the completed work on secondary temperature standards, a value of 2053°C (IPTS) for the melting point of alumina ( $\alpha$ -Al<sub>2</sub>O<sub>3</sub>) can be recommended.

*Task Force on Secondary Temperature Standards.* (A detailed publication is being prepared.) Work on the melting point of alumina has been completed. Overall, 8 groups representing 7 countries participated in the experimental portion of the endeavor. A summary report has been received from the Task Force from which the following is abstracted.

In order to obtain maximum participation only a minimal number of controls was established for individual melting point experiments. The broad guidelines were limited to: (a) utilization of a common sample, (b) tungsten containers, and (c) no restriction on equipment or technique.

The central source of Al<sub>2</sub>O<sub>3</sub> was prepared from stock alumina by fusion in a solar furnace, thus minimizing the possibility of contamination from extraneous sources. The primary supply of Al<sub>2</sub>O<sub>3</sub> was prepared and distributed by Dr. M. FOEX (France). Individual lots distributed to Task Force members consisted of 400-500 g of large conglomerates of polycrystalline



$\text{Al}_2\text{O}_3$ . X-ray patterns of the material showed only reflections identifiable with  $\alpha\text{-Al}_2\text{O}_3$  (corundum type). All grinding or other processing was left to the discretion of the individual Task Force member. As indicated by spectrochemical analyses, the alumina samples had a nominal purity of at least 99.9%.

As expected, the experimental techniques and equipment employed by the different investigators varied in several respects, with no two groups exactly duplicating one another. With one exception, all utilized optical pyrometry for temperature measurement. Furnace types included resistance, induction, and solar. Environmental conditions ranged between high vacuum and air or argon at various pressures. Both static and dynamic methods were used and included the traditional thermal analysis technique, a modified quench method, and the less conventional direct observation procedure.

Each method, of course, has attendant problems peculiar to the specific procedure. Perhaps the greatest difficulty inherent with any method is the measurement of temperature. In most instances, the entire temperature measurement system was calibrated before actual  $\text{Al}_2\text{O}_3$ -point determination using two or more known reference points: Au 1063°C, Pd 1552°C, Pt 1769°C, or Rh 1960°C (ITS 1948). In addition, all pyrometers and thermocouples were separately calibrated by approved techniques.

The melting points of  $\text{Al}_2\text{O}_3$ , as determined by the individual Task Force members, are listed in the table. Each melting point is an average of several separate determinations. The listed precision and accuracy are based largely on the specific investigator's personal estimate.

Measured Melting Points of  $\text{Al}_2\text{O}_3$

Melting Point ITS 1968, °C	Accuracy, °C	Precision, °C
2043	±2	±2
2045	6	3
2054	3.6	0.8
2054	7	3
2054	6	2
2054	4	1
2055	6	2.5
2055	6	1.5
2073	15	9

The overall average of the 9 separate reported average melting points is 2054°C (ITS 1968) with a standard deviation calculated to be 8.4°C. Each of the reported melting points was obtained through the use of an integral system of equipment and procedures and generally involves the personal judgment of the investigator. Unless there is a true or absolute value available for comparison, deletion of any one set of data might not be completely justified. However, if the 2073°C (ITS 1968) is excluded from consideration on the basis of a statistical treatment, the overall average value becomes 2052°C (ITS 1968) with a standard deviation of 4.8°C. The rejection of both extreme values, 2043°C and 2073°C (ITS 1968), reduces the grand average only by one to 2053°C (ITS 1968), while the standard deviation is substantially reduced to 3.6°C. On the basis of these data the melting point of  $\text{Al}_2\text{O}_3$  apparently is between 2051°C and 2053°C (ITS 1968). *Since errors associated with melting point determinations generally yield lower than true values, it*

would appear that a value of  $2053^{\circ}\text{C} \pm 4^{\circ}\text{C}$  (IPTS 1968) is a realistic figure for the alumina point. For comparison it should be noted that the average melting point for all determinations published since 1948 is  $2047^{\circ}\text{C}$  (IPTS 1968) with a standard deviation of  $11.4^{\circ}\text{C}$ .

The cooperative effort reported here has demonstrated that it is technically feasible to determine the melting point with sufficient precision to warrant its use as a temperature standard. Therefore, it is proposed that the Commission recommends to the Advisory Committee on Thermometry that it take appropriate action to include the alumina point as a secondary reference point on the International Practical Temperature Scale.

The Task Force is planning additional work on other materials for secondary temperature standards. The Commission will consider similar measurements on other oxides such as yttrium oxide ( $\sim 2400^{\circ}\text{C}$ ) and possibly zirconium oxide ( $\sim 2800^{\circ}\text{C}$ ) as well as on refractory metals such as Re and W.

*Task Force on Vapor Pressure Standard Reference Materials.* This program was established to provide 5 vapor pressure standard reference materials which will cover a pressure range of  $10^{-3}$  to  $10^{-8}$  atm over a temperature range of  $100$ - $3000^{\circ}\text{C}$ . The materials chosen are Cd, Ag, Au, Pt, and W. The techniques normally used to measure vapor pressures over these ranges are the Langmuir, Knudsen, torque Knudsen, and mass spectrometric techniques. Standard reference materials are needed to allow workers in the field to determine the accuracy and precision of their apparatus and techniques. The accuracy of vapor pressure measurements needs to be evaluated since experience has shown that large systematic errors in high temperature vapor pressure measurements are not uncommon.

A total of 30 laboratories cooperates with NBS. A vapor pressure certificate will be issued for each material and samples will be made available to the public. The Au sample is the first such material. Processing of the Cd and Ag data has now been started.

A detailed statistical analysis has been made of the Au data, and heat of vaporization and P-T values have been selected (a complete technical report is being prepared). These results use new heat capacity data for liquid Au which have been obtained by one of the cooperating laboratories. The heat capacity data significantly improve the existing thermodynamic functions for liquid Au.

The most probable value of the heat of sublimation of solid gold at  $298\text{K}$  indicated by the data is  $367040$  joules ( $87720$  thermochemical calories) per mole. The most probable values of the equilibrium vapor pressure of gold are given in the following table.

Temperature	Vapor Pressure <sup>2</sup>
1300K	$9.76 \times 10^{-9}$ bar
1338, m pt <sup>1</sup>	$2.52 \times 10^{-8}$
1500	$7.24 \times 10^{-7}$
1800	$7.15 \times 10^{-5}$
2100	$1.85 \times 10^{-3}$

<sup>1</sup> International Practical Temperature Scale of 1968 uses  $1064.43^{\circ}\text{C}$  for the gold point.

<sup>2</sup> One atmosphere =  $1.01325$  bar.

*Working Group on Bibliographies* (Dr. J. J. DIAMOND, Coordinator). The Working Group continues to function efficiently and has compiled and pub-

lished its bibliographies every three months without fail. Several changes have been made recently. First, the separate bibliographies on materials in the condensed state and on gases and plasmas have been combined into a single bibliography. Second, coverage of research on refractory materials at temperatures below 1000° has been discontinued. Finally, it was found to be impossible to continue the 11-year practice of distributing the bibliographies free, and they are now sold for the cost of printing by US Government Printing Office. The cost of editing and preparing each issue for printing continues to be underwritten by NBS.

A study is being made on the use of a computer as an aid in the preparation of the bibliography. The current emphasis is on an attempt to use computer tapes generated by the Chemical Abstracts Service as an aid in searching the literature.

*Other Activities.* Further enquiries are being directed to active scientists in other fields of high temperatures and refractories, such as carbon research and high temperature mass spectrometry, in particular the problem of ionization cross sections.

Dr. WALKER was Vice-General Chairman for the Asilomar Conference, Pacific Grove, September 1967. The meeting was under IUPAC patronage.

Dr. Horton represented IUPAC at the *International Symposium on the Reactivity of Solids*, Schenectady, August 1968.

#### **4. Future Plans**

With respect to the melting point standards the Commission will consider similar measurements to those carried out for alumina on other oxides, particularly yttria and in a second step on zirconia. Serious consideration is being given to the desirability of measurements of the melting point of refractory metals, particularly platinum. Contact with the appropriate groups in IUPAP will be made.

The Task Force on Vapor Pressure of Standard Reference Materials will be continued. Activity should be extended to subjects such as measurement of the triple point of carbon, precise measurements of diffusion coefficients in solid state materials at high temperature, and cooperative measurements of ionization cross section for high temperature gaseous species.



# ORGANIC CHEMISTRY DIVISION COMMITTEE

3rd and 6th July 1969

*Present:* Prof. P. D. BARTLETT (in the chair), Prof. D. H. R. BARTON, Prof. G. OURISSON, Prof. V. HEROUT, Prof. A. KJAER, Prof. K. NAKANISHI, Prof. P. YATES, Prof. H. ZOLLINGER.

At the open meeting on 3rd July, Prof. S. RANGASWAMI was present as an Observer; on 6th July, Profs. W. KLYNE, S. VEIBEL, T. URBANSKI, and O. HOFFMANN-OSTENHOFF, and Dr. R. MORF were present.

## I. Membership of Division Committee

Profs. HEROUT and ZOLLINGER have been re-elected for a period of 4 years. Prof. BARTON took up, at the second meeting, the Presidency of the Division until 1971. Prof. OURISSON was elected Vice-President (President-elect) to take up the Presidency of the Division in 1971. Prof. KJAER was elected Secretary until 1971.

These elections were submitted to Council for approval. In the two vacancies left by Profs. WEYGAND and NAKANISHI, the Committee elected Prof. M. NAKAJIMA (Japan) and Prof. J. ROMO (Mexico).

## 2. Commissions

*Commission III.1.* (a) The Committee discussed the report submitted by Prof. VERKADE. Several Members expressed the view that, besides the classical types of verbal nomenclature, it might soon become necessary to consider also the various types of nomenclature needed for computerized literature searches. The need for such a prospective approach to nomenclature problems should influence the nominations for the next vacancies on the Commission.

The Committee suggested that the Commission should consider approaching practising organic chemists having shown an active interest in nomenclature problems, not necessarily along the lines of the work of the Commission. Prof. VERKADE has explicitly mentioned that he will not stand for re-election after his present term expires in 1971. The Division Committee suggested that Prof. V. PRELOG (Switzerland) might be convinced to replace him as Chairman of the Commission. As potential new Members, the Committee further suggested the names of Dr. K. HIRAYAMA (Japan) and of Prof. A. DREIDING (Switzerland). All three could already be invited by the Commission as Associate Members. Prof. KJAER will be responsible for conveying these suggestions of the Division Committee to the Commission.

(b) The Commission had suggested the nomination of Dr. K. BLAHA (Czechoslovakia) as an Associate Member. The Division Committee approved this nomination.

(c) The Division Committee recommended publication of:

*Section D of Nomenclature of Organic Chemistry*, as a joint publication of the Inorganic and Organic Chemistry Divisions.

*Sections A, B and C*, in their revised version, when the manuscript is finalized.

*Commission III.2.* (a) The President's report for 1969, based on the information obtained from the Commission, stated that the activity of this Commission appeared to be low, and that its dissolution might be considered. The excellent report of the Commission, which met for the second time in Cortina, made it clear that much of the activity of the Commission had remained rather confidential, but that its aims were progressively and satisfactorily

fulfilled. The nature of the problems remaining, notably in the field of documentation and abstracting, makes it highly desirable to let this Commission pursue its work at least for another term of 2 years. The Division Committee expressed the wish that the activities of this Commission be made more clearly known in its yearly reports in future.

(b) The Division Committee approved the nominations to the Commission of Dr. T. MABRY (USA) and Dr. J. B. HARBORNE (UK) to replace Prof. MARION and Dr. BATE-SMITH. The Commission has elected Prof. KJAER as Chairman and Prof. SWAIN continues as Secretary, both subject to approval by Council.

(c) Should another vacancy appear in the Commission before the next IUPAC Conference, the Division Committee suggested that the Commission could nominate Prof. S. NATORI (Japan).

(d) The Committee approved the proposal of the Commission to organize a *Symposium on Chemistry and Biosystematics* in Strasbourg in 1971.

(e) The Division Committee approved the plans of the Commission to meet in Copenhagen in June 1970, and to allocate the Commission \$2,500 for 1970.

*Commission III.3.* This is a Joint Commission of IUPAC and IUB, and the Division Committee has still to find out in what respect it is controlled by the appropriate units of the two Unions, as far as its scientific work goes.

(a) The Division Committee recommended publication of the nomenclature rules of *Carbohydrates* and *Carotenoids*, as tentative nomenclature rules, as soon as the manuscripts are available.

(b) The Division Committee recommended setting up a small committee formed of Members of Commissions III.1 and III.3, to review the nomenclature rules on diterpenes prepared by a group headed by Dr. J. W. ROWE (USA) and to prepare them for publication as tentative rules of IUPAC.

(c) The Division Committee recommended that the group entrusted with the revision of nomenclature rules for amino-acids considers also the various non-protein natural amino-acids.

*New Commissions.* (a) *Photochemistry.* The Committee had for some time felt the need for standards to be applied to work and to publications in the field of photochemistry. An *ad hoc* Committee had been set up, which has now made specific recommendations as to the terms of reference under which a new Commission on Organic Photochemistry should be appointed. The Division Committee has approved this report (see *Annex*) and proposed to the Bureau and further to Council that this new Commission be established. The first Officers of the Commission should be Prof. G. S. HAMMOND (USA) as Chairman and Prof. G. QUINKERT (Germany) as Secretary.

(b) *Medicinal Chemistry.* The case for inclusion of a Commission on Medicinal Chemistry was discussed at length, and compared with the merits of the establishment of a Section on Medicinal Chemistry, attached either to the Bureau or to the Organic Chemistry Division.

The proposal by the Bureau to attach a Section on Medicinal Chemistry to the Organic Chemistry Division was approved, with Prof. E. CAMPAIGNE (USA) as Chairman and Dr. L. STERNBACH (USA) as Secretary.

However, this new Section is in conflict with the present organization of the Division; this point is discussed below (see Item 4). On the basis of expert advice solicited during the Conference, and to avoid unnecessary duplication of effort, the Committee assumes that *Medicinal Chemistry* is to be accepted as the English equivalent of *Chimie Therapeutique* in French and *Pharmazeutische Chemie* in German, even though there may, of course, be nuances in the implications of these names.

### 3. Sponsorship of Symposia

*Approved Symposia.* The Committee noted with pleasure the approval by the Bureau of the following symposia:

Conformational Analysis—Bruxelles (1969)  
Cycloaddition—München (1970)  
Nonbenzenoid Aromatic Compounds—Sendai (1970)  
Carbohydrates—Paris (1970)  
Photochemistry—St. Moritz (1970)  
Natural Products—Riga (1970)

in some cases, subject to clarification of pending problems.

As regards the *Symposium on Natural Products* in Riga, the requested subvention of \$7,500 had been reduced by the Bureau to \$2,500. The budget submitted by the organizers appeared to be unsatisfactory. A careful check on the needs of this symposium, to cover approximately the travel of the invited speakers to and from Moscow, shows that a minimal subvention of \$5,000 is absolutely justified. The Division Committee asked the Bureau to reconsider its position on the matter.

*New Symposia.* (a) *Symposia within 1971 IUPAC Congress in Boston.* The Committee suggested the inclusion of symposia on the following themes:

Biosynthesis  
Insect Chemistry  
Stereochemistry of Sulphur-organic Compounds.

Prof. BARTLETT will ask the Organizing Committee of the Congress to consider how to implement these suggestions.

(b) *Symposia on Chemistry of Natural Products.* There is every reason to believe that, after the Riga meeting, another symposium will be planned in this highly successful series, for 1972. The Committee suggested that this symposium could be held in Delhi, subject to approval by the Adhering Organization from India, and to the necessary steps being undertaken by a suitable group of Indian chemists, of whom Prof. S. RANGASWAMI and Dr. T. R. GOVINDACHARI had already shown great enthusiasm.

The Committee decided to ask Prof. SHEMAKIN, as one of the organizers of the Riga symposium, to refer to the President of the Division Committee any other suggestion he would get for possible locations of the next symposium.

(c) *Symposium on Organic Solid-State Chemistry* (Israel). The Division Committee approved this symposium.

(d) *New Series.* As mentioned in the President's report presented to Council, the Committee had previously contemplated, and wished now to recommend, setting up two new regular series of organic chemistry symposia, to be held at 2-yearly intervals in non-Congress years:

*Symposia on Physical Organic Chemistry* (including reaction mechanisms). The first symposium might be organized in Switzerland in 1972.

*Symposia on Synthetic Methods of Organic Chemistry.* The first symposium might be organized in Zürich (Switzerland) in 1974 under the responsibility of Prof. C. H. EUGSTER.

### 4. Other Business

*Sectional Structure vs. Commissions.* At its meeting in Prague, the Division Committee had considered that its work was best done at three levels:



- (a) the Committee meetings (with associated mail work),
- (b) the work of the Commissions,
- (c) symposia carefully planned to cover the most important branches of organic chemistry.

The Committee had rejected the idea of organizing the Division in permanent units covering adequately the whole field of organic chemistry.

The decision of the Bureau to set up a Section on Medicinal Chemistry caused the Committee to revise its stand. If such a Section was anyway created, then its place was certainly within the Organic Chemistry Division, and the Division Committee should be responsible for helping this new Section to be a useful and efficient segment of the Division (*cf.* Item 2).

This change had led the Division Committee to discuss again the question of a sectional organization. This was considered to be not an advisable organization for the time-being. Future requests for new Commissions or new Sections will be considered on their own merits; if too many Sections were proposed, the Committee would have to reconsider completely the organization of the Division.

*Duties of Division Officers.* A short draft had been prepared, to clarify the various duties of the Officers of the Committee.

*Publications.* A memorandum prepared by Prof. E. A. SHILOV, calling for the suppression of publication of micro-analytical data, had been discussed by mail within the Committee. No agreement had been reached. A direct discussion had now led to the following conclusions.

The waste of space due to inclusion of C,H-analyses is minor compared to the magnitude of the problem of the increasing volume of publications. In most cases, the publication of such data can serve as an independent criterion for the quality of the experimental work involved, and may provide future workers with important indications leading not infrequently to revisions of wrong interpretations. Other analytical data such as spectra, usually serve other purposes, but can rarely be used to replace elemental analyses, which anyway now require sub-milligram amounts of substances.

For all these reasons, the Committee was not in favour of giving IUPAC support to an appeal to editors to relax their present invites calling for inclusion of C,H-analyses.

Any relaxation of these rules should anyway not take the form, now usual: 'All the compounds described have given satisfactory analytical values', but any such wording should include a statement of the acceptance bracket, *e.g.*, 'All the compounds for which a molecular formula is provided have given analytical values in agreement with that molecular formula, according to Gysel, within 0.2%.' Substances not so covered should be described completely.

Again, the Division Committee had discussed the problems associated with the *explosion of information*. The Committee would be ready to consider a proposal, under which *every* chemical publication would be in a shortened form (*e.g.*, 1-2 printed pages), this being accompanied by a complete manuscript prepared in the now usual way and deposited but not published *in toto*. Such a scheme would only be acceptable if ways were found:

- (a) to ensure critical refereeing, not only of the published extended summary, but also of the complete manuscript;
- (b) to ensure prompt and cheap distribution of the complete manuscript to anyone interested;
- (c) to ensure abstracting of the complete manuscript.

All this required further study. The Secretary was instructed to consult editors of leading journals on this problem.

**Resolution.** The Division Committee resolved:

that in all activities in which it is desirable for IUPAC Committees, Commissions, Sections, or Divisions to collaborate with other international organizations, any special IUPAC rules which operate against such collaboration should be waived.

**Next Meeting.** The Division Committee will meet in Munich on 12-13th September, 1970.

### **Annex—Proposal for a Commission on Organic Photochemistry**

During the last 15 years there has been a remarkable growth in the subject of organic photochemistry. Indeed, at the present time, this subject represents one of the major activities of organic chemists. There have been two international meetings sponsored by IUPAC devoted to organic photochemistry, and a third will take place in St. Moritz next July. There is every reason to believe that these meetings, which have had no difficulty in finding financial support outside of IUPAC assistance, will continue to be held every 3 years.

At the II<sup>nd</sup> IUPAC meeting on organic photochemistry, held in the Netherlands in 1967, a number of the leading experts in the field found, through mutual discussion, that there were many general problems, such as nomenclature, units, specification of standards, as well as certain problems of practice, like the criteria for identification of excited states, the measurement of quantum yields, the standardization of filters, *etc.*, which required expert international discussion and agreement.

The Organic Chemistry Division Committee proposes, therefore, that a new *Commission on Organic Photochemistry* should be created to deal with these problems. The Members of this Commission might include one or two physical chemists, among them an expert spectroscopist, so as to ensure that the recommendations of the Commission should, as far as possible, be reconcilable with current practice in physical chemistry.

A joint committee between the Commission on Organic Photochemistry and the appropriate Commissions on Physical and Analytical Chemistry would also be needed at some time in the future, to finalize the recommendations made by the Commission on Organic Photochemistry.

It is proposed that Prof. G. S. HAMMOND (USA) should be invited to be Chairman of the new Commission, with Prof. G. QUINKERT (Germany) as Secretary. The Commission should be created, with a reduced membership, in time to hold a meeting during the *III<sup>rd</sup> International Symposium on Organic Photochemistry* in St. Moritz (July 1970).

## COMMISSION III.2: CHEMICAL PLANT TAXONOMY

1. The Commission was established in 1965, but due to economic reasons, had only met in Stockholm (28-29th June, 1965) before the present meeting in Cortina d'Ampezzo on 3rd July. The following Titular Members were present: MARION, SWAIN, BATE-SMITH, ERDTMAN, KJAER, OURISSON.
2. At its first meeting the Commission had set itself four main tasks: *viz.* documentation, standards for chemotaxonomic publications, library of reference compounds, identification and storage of plant specimens.
3. The problems of documentation are particularly difficult in the field of chemical plant taxonomy due to its interdisciplinary nature. Abstracting journals are disinclined to give prominence to reports of the occurrence of already known compounds found in hitherto undescribed sources and such information is often missed out when abstracts are encoded for use with computer-based information storage and retrieval systems. Furthermore, some biological abstracting journals occasionally ignore reports of the isolation of new compounds unless they have apparent biological significance.
4. With the increasing interest in this widening field, which the Commission feels its formation has in great part engendered, it is particularly important that relevant information in the literature (including that in biochemistry, microbiology, zoology, and molecular biology) is properly abstracted and readily retrievable for use.
5. The Commission concentrated its efforts first on the possibility of continuing, broadening, and bringing up-to-date, a Japanese publication *The Annual Index of the Reports on Plant Chemistry* edited by Prof. KARIYONE. The Commission contacted the Japanese publisher and also Butterworths (the official IUPAC publisher). The Commission also approached several other publishers in France, UK, and USA to see if commercial interest could be roused in the project. Unfortunately, such interest is lacking at present.
6. The Commission had also made contact with the main abstracting organizations including some commercial services. These negotiations are still continuing but the Commission believed that it can most usefully proceed by using its influence to persuade abstract services of the need for wider coverage in the field. To demonstrate the extent of the difficulties, the Commission had arranged for a small pilot study to be carried out by the Kline Science Library, Yale University, through the courtesy of the librarian (Mr. J. HARRISON) and the Yale Corporation.
7. The Commission was of the opinion that the standards of publication dealing with chemical plant taxonomy were generally low and this led to their being rejected by editors of appropriate journals. Accordingly, the Commission devised a format for short papers reporting chemotaxonomic information. This format has been accepted by *Phytochemistry* and several other journals.
8. The Commission investigated the possibility of the establishment of a library of reference compounds based on the collection of Prof. C. MENTZER in Paris. Unfortunately, Prof. MENTZER died while negotiations were in an early stage. In view of the fact that other attempts of this kind which were reported to the Commission do not appear to have been successful, the Commission decided not to pursue the matter further at the moment.
9. The Commission took note that many of the reports of the occurrence of natural products are marred by the fact that authors are either not punctil-



lious or, more generally, ignorant of the need for accurate plant identification and to deposit voucher specimens in designated Herbaria, at least of the rarer species. In collaboration with its sister organization, the International Association of Plant Taxonomists (IAPT) Committee on Chemotaxonomy, the Commission had drawn up a set of rules to be followed. The IAPT Committee has been preparing a list of suitable Herbaria and when this is complete, the Commission will circulate the recommendations and list to interested international and national journals.

10. The Commission has taken note that since its inception, 6 major international meetings in the general area of chemotaxonomy (or biochemical systematics as the widening field is becoming known) have been held. Most of these have concentrated on biochemical and macromolecular aspects of the field, and several have been published in book form.

11. The Commission noted with pleasure that the *Chemical Taxonomy Newsletter* which is now sponsored jointly by the University of Texas (edited by Dr. T. MABRY) and the University of Reading (edited by Dr. J. B. HARBORNE) has continued to flourish as a forum for the publication of important articles in the area, and now has a circulation approaching 500 members.

12. The Commission noted with regret the deaths of Prof. CHARLES MENTZER (Musée Nationale d'Histoire Naturelle, Paris) and Prof. R. ALSTON (University of Texas; Secretary of the IAPT Committee), both of whom had given their help generously to the Commission.

13. The Commission also noted with regret that Prof. MARION and Dr. BATE-SMITH have tendered their resignation as from 31st July, 1969. Their guidance and wise counsel will be greatly missed.

14. The Commission believed its work is far from done. There is still a need to ensure that closer links are forged between the Commission (representing the chemists) and representatives of the botanists, zoologists, and biochemists (including molecular biologists). The Commission believed that this can best (and perhaps only) be done under the auspices of an international organization such as IUPAC. If IUPAC does not take the lead, the Commission believed that other organizations will do so. The Commission recommended, therefore, that its objectives should continue to be the responsibility of the Organic Chemistry Division.

15. There is also the extremely important question of continued studies on documentation. Here the Commission believed that without its authority, continuing studies in the field of information storage and retrieval of interest in biochemical systematics will not readily proceed. The Commission understands, for example, that the studies by the Kline Library, Yale University, would probably be terminated unless the Commission showed continued interest. It seemed probable that the Library might obtain some grant from Government or private foundations to extend this work. Similarly, the Commission believed that the initiation (and continuation) of the discussions with the abstracting services would be impossible if the Organic Chemistry Division had not taken this initiative of establishing the Commission. They recommended, therefore, that all these activities continue.

16. The Commission further recommended that the time is now ripe for the planning and organization of an international symposium in the field under the auspices of IUPAC. Such a symposium should take note of the recent advances in the field and this will mean ensuring that proper links are maintained with the appropriate bodies in botany, zoology, and biochemistry.

17. The Commission recommended that Dr. J. B. HARBORNE and Dr. T. MABRY be invited to accept invitations as Titular Members of this Commission on the resignations of Prof. MARION and Dr. BATE-SMITH. The Commission further recommended that Prof. KJAER be appointed Chairman as from 1st August, 1969.

# MACROMOLECULAR DIVISION COMMITTEE

*1st July 1969*

*Present:* Prof. O. WICHTERLE (in the chair), Prof. H. BENOIT, Prof. G. SMETS, Dr. J. W. BARRETT, Prof. O. HORN, Prof. C. G. OVERBERGER (Titular Members); Dr. R. W. CAIRNS, Prof. M. LETORT (Associate Members); Dr. I. M. PANAYOTOV, Prof. A. BJORKMAN, Dr. J. DE VRIES, Dr. F. ENGEL, Prof. A. SILBERBERG, Prof. A. J. STAVERMAN, Dr. F. J. JOUBERT (National Representatives); Prof. H. A. SCHERAGA (Representative of IUPAB); Prof. K. A. WOLF (Representative of IUPAP).

*Apologies for non-attendance:* Prof. S. S. MEDVEDEV, Prof. S. OKAMURA, Prof. G. V. SCHULZ.

*In attendance:* Dr. K. L. LOENING, Prof. G. SCHAY, Dr. C. SUHR.

## I. Minutes

The minutes of the previous (IIInd) meeting in Frankfurt-Höchst on 2nd March, 1968, and of the informal (IIIrd) meeting in Toronto on 4th September, 1968, were approved.

## 2. Membership

The additional By-laws for elections within the Division which were proposed in the 1st Division Committee meeting in Brussels (11-12th November, 1967) were rediscussed and amended as follows:

- (a) The date of rotation of Titular and Associate Members should coincide with the date of an IUPAC Conference.
- (b) Every 2 years half of the Titular Members should be renewed.
- (c) The maximum period of Titular Membership is 4 years with only those exceptions which follow from the general By-laws of IUPAC.
- (d) The names for election as new Titular and Associate Members should be collated about 1 year in advance from all Members and National Representatives of the Division. A complete list of candidates should be sent to all Members of the Division for preliminary election. By this procedure a priority list will be established and submitted for renewal elections.
- (e) These rules will be applied starting from the XXVIth IUPAC Conference in 1971.

## 3. Activities of Division

Reports from Dr. LOENING's Commission on Macromolecular Nomenclature, from Dr. BARRETT's and Professor BENOIT's Working Groups on Properties and Structure of Commercial Polymers, and Professor SMETS's report on Teaching in Macromolecular Science were submitted for discussion and approved by the Committee. All these activities will continue in the sense as resulting from these discussions.

## 4. Scientific Meetings

IUPAC sponsorship was recommended for the Leiden symposium in September 1970. Prof. STAVERMAN, Chairman of the Scientific Committee of this symposium, gave a report on the preparations. Similarly, Prof. SCHAY commented about the last steps of preparation of the Budapest symposium in August 1969.



A Gordon-type discussion meeting on *Models of Biopolymer Structure and Functions* was recommended for further consideration and for joint sponsorship by IUPAC and IUPAB.

Dr. BARRETT asked for sponsorship of a public conference on *Molecular Relaxation Phenomena and Physical Properties of PVC* in connection with the activity of his Working Group. The Bureau will be asked for advice on sponsorship either by IUPAC or by the Macromolecular Division.

### **5. Contacts with Other Unions**

(a) *IUPAB*. Prof. SCHERAGA will consider within IUPAB the possibility of the joint meeting mentioned above. He will also assume further liaison between IUPAB and IUPAC.

(b) *IUPAP*. Considering that the Division must continue to deal adequately with macromolecular science and technology because of the impossibility of separating chemical and physical contributions, the Division will ensure that its membership is maintained as representative of the various disciplines serving macromolecular science and technology. Prof. WOLF as representative of IUPAP will assume contacts with the polymer physics groups organized in USA, Japan, Germany, and some other countries.

# **ANALYTICAL CHEMISTRY DIVISION COMMITTEE**

*30th June and 3rd July 1969*

*Present:* Prof. P. W. WEST (in the chair), Prof. W. KEMULA, Mr. R. W. FENNELL, Prof. R. BELCHER, Prof. C. DUVAL, Prof. L. ERDEY, Prof. T. FUJINAGA, Prof. D. N. HUME, Prof. H. KAISER.

*In attendance:* Dr. R. MORF (in part)

## **1. President's Opening Remarks**

The President said that he thought the Division to be in a good state and generally to be running smoothly, although there were still some organizational problems to be overcome. He then welcomed the presence of the Secretary General at the meeting and invited him to speak to the Committee.

Dr. MORF paid tribute to the work of the Division and said that it has and will play a major role in the work of IUPAC. The influence and scope of the Division had been steadily increasing since its formation and he was sure that this trend would continue.

## **2. Minutes of XIth Division Committee Meeting**

The minutes as published in *Comptes Rendus XXIV Conference* were approved.

## **3. Election of Committee Members**

(a) *Report of Nomination/Election Committee (1967-69)*. Mr. FENNELL, on behalf of Dr. ZUMAN, Chairman of the N/E Committee, presented a report on the election of 3 Committee Members. The newly elected Members were:

Prof. W. FISCHER (Germany)

Prof. H. FREISER (USA)

Prof. N. TANAKA (Japan)

The President expressed his gratitude to the Members of the N/E Committee for their work.

(b) *Election of N/E Committee (1969-71)*. The Committee proposed that the following be invited to serve on the N/E Committee for 1969-71: Dr. A. A. SMALES (Chairman), Prof. C. T. J. ALKEMADE, Prof. L. B. ROGERS. In case of difficulty, the Division Executive Committee is empowered to invite alternative Members.

## **4. Proposals of USSR Adhering Organization**

(a) *Unification of Analytical Techniques for Determination of Minor Amounts of Impurities in High-grade Chemicals*. This proposal had been brought to the attention of Commission V.2 by the President.

(b) *Recommended Set of Organic Reagents for Detection of Inorganic Ions and Functional Groups in Organic Compounds*. The attention of the USSR Adhering Organization had been drawn to the report *Reagents and Reactions for Qualitative Inorganic Analysis (Pure and Applied Chemistry* **8**, 1 (1964)). Further work could be taken up by Commission V.1 only when the work on the CE cooperative programme had been sufficiently well established.

## **5. Consideration of Reports from Commissions**

Mr. FENNELL presented 2 reports from Commission V.3 which required Division Committee approval:

(a) *Recommendations on Ion Exchange Nomenclature*. The report was approved for submission to Council for publication as tentative nomenclature rules.

(b) *Recommended Terminology for Automatic Analysis*. After some discussion it was agreed (6 votes for, 1 against) that the report should be submitted to Council for publication as final nomenclature rules.

Prof. KAISER expressed his concern about the production of nomenclature reports by IUPAC. He suggested that the reports must have a sound logical and etymological basis as well as being scientifically correct and queried whether IUPAC Commissions were constituted so as to achieve this. It was agreed that IUPAC recommendations on nomenclature must be of a high standard and that Prof. KAISER's comments must always be borne in mind.

Dr. MORF stated that reprints of tentative recommendations published in the *Information Bulletin* could be ordered by Commissions to send to persons likely to be interested who did not receive the *Bulletin*.

## 6. Teaching in Analytical Chemistry

Prof. HUME stated that he had reconsidered the documents in his possession and had finally decided that the most appropriate way to present the information was perhaps in the form of a report. This report was presented to the Division Committee and it was agreed that the Members should send their comments to Prof. HUME by the end of October.

## 7. Division Finances

Mr. FENNELL summarized the returns made for funds in 1970 and 1971. Meetings had been requested by Commissions V.3 (1 day) and V.4 (3 days) and the Officers of Commissions V.3 and V.5 wished to meet those of Commissions I.1 and I.3. Commission V.2 requested permission to hold a meeting in 1970 in Graz but without IUPAC subvention. In addition, it had been proposed that the Division Executive Committee should also meet in Graz (2-3 days).

All Commissions wished to meet at the IUPAC Conference in 1971.

The *ad hoc* Committee on Nomenclature in Analytical Separation Processes requested funds for a meeting in 1970.

Prof. KEMULA would require funds for secretarial expenses during his term of office as Division President. Prof. WEST stated that in 1969 a contingency fund (\$2,000) had been allocated to each Division President to use at his discretion in order to advance the work of his Division.

## 8. Sponsorship of Symposia

Mr. FENNELL reported that the Division had recommended IUPAC sponsorship for 3 meetings:

(a) *Symposium on Non-Aqueous Electrochemistry*, Paris, 8-10th July, 1970. IUPAC sponsorship had been granted provided that specially invited lectures would be published in *Pure and Applied Chemistry*.

(b) *IIIrd Analytical Conference*, Budapest, 24-29th August, 1970. IUPAC sponsorship had been granted with the publication proviso mentioned above.

(c) *International Congress on Analytical Chemistry*, Kyoto, 3-7th April, 1972. IUPAC sponsorship had been granted with the publication proviso. Prof. FUJINAGA distributed copies of the preliminary announcement and hoped that it would be possible for the Division Executive Committee to meet during the Conference.



Prof. KAISER queried the basis on which sponsorship was given and the Secretary outlined the procedure agreed by the IUPAC Executive Committee. It was pointed out by Prof. KAISER that if only the plenary lectures were published, the procedure, which referred to publication of the proceedings, was misleading.

## **9. Cooperation with Other International Organizations**

Mr. FENNELL referred to the ICSU Committee on Data for Science and Technology, in which IUPAC was represented, and said that he had asked that *CODATA Newsletters* should be sent to the Chairman of Commissions concerned with compilation of data.

The Secretary drew attention to Prof. KAISER's work with the ICSU/UNESCO Joint Project on the Communication of Scientific Information. Prof. KAISER outlined the problems involved in the evaluation and codification of information.

Prof. WEST outlined the proceedings of a meeting held under the auspices of the International Union against Cancer and the International Agency for Research on Cancer which was concerned with the analytical chemistry of inorganic carcinogens. The report of the meeting had been submitted to WHO. Finally, Prof. WEST forecast that the Division would be increasingly consulted on international problems in the future.

## **10. International Laboratory for Analytical Chemistry**

This item had been discussed at the Open Meeting of the Division and a proposal drafted for consideration by the Bureau (see Report of the Open Meeting: Item 4 and Appendix). It was agreed that if the Bureau approved the setting up of the Working Group, the following should be invited to become Members—Prof. R. BELCHER, Dr. H. EGAN, Prof. T. FUJINAGA, Prof. H. KIENITZ, Prof. H. MALISSA, Dr. W. W. MEINKE, Prof. J. MINCZEWSKI, Prof. J. ZÝKA, Dr. H. MERTEN (IAEA), and one representative each from USSR, ILO, and UNIDO. It was agreed that Prof. MALISSA be invited to act as Chairman of the Group and that the Chairman should have the power to coopt further Members if required.

## **11. General Rules of Division**

Mr. FENNELL explained that the draft rules he had drawn up and circulated were an attempt to up-date the rules previously published in 1962 and had been framed to provide as much information as possible so that the routine administrative tasks of the Division could be accomplished without difficulty.

Comments and proposals from Members of the Division were considered and various amendments made. These will be incorporated into a further set of rules for which Council's approval will be sought.

The more important proposals were:

*Rule I. 1 (ii).* It was proposed by Prof. BELCHER, seconded by Prof. KAISER, and carried unanimously 'that the Division Secretary should not be included amongst the 10 Committee Members entitled to vote, and that he should be elected without regard to zonal representation.' Because this would mean that the Division Committee would then consist of 10 voting Members and 1 non-voting Secretary, the approval of the Bureau would be sought under By-law 4.102 to bring this rule into effect for the elections in 1971.

*Rule I. 1 (iii).* Add at end 'Newly elected Members may attend Division Committee meetings as Observers before their term of office begins.'

*Rule I. (iv).* It was proposed by Prof. BELCHER, seconded by Prof. HUME, and carried unanimously that 'or in a . . . . . August 1st' be deleted and the following be added: 'In the event of the resignation or death of a Committee Member more than one year before the expiry of his term of office, the Division Executive Committee is empowered to make a temporary appointment tenable until a normal election for the relevant zone has taken place.'

*Rule V.* Publication of Commission Reports. This item was discussed at the Open Meeting of the Division and a proposal drafted for consideration by the Bureau (see Appendix A of the Report of the Open Meeting).

## **12. Programmes of Commissions**

Commission Chairmen who were not Members of the Division Committee had been invited to attend the meeting during discussion of this item.

(a) *Status Reports.* The status reports of the Commissions had been circulated to the Division Committee.

(b) *Programmes 1969-71.* The programmes of the Commissions were discussed and, after some amendment, were approved. It was noted that a number of Commissions were concerned with trace analysis and/or the purity of materials. Although there appeared to be no overlap of interests at the moment, it may soon become necessary to set up an inter-Commission Committee to coordinate this type of work.

(c) *Membership 1969-71.* The membership proposals of the Commissions were approved with the addition of Dr. G. INGRAM (UK) to Commission V.2.

## COMMISSION V.1: ANALYTICAL REACTIONS AND REAGENTS

### 1. Meeting

The Commission met on 1st and 2nd July. The following Titular Members were present: MALISSA, BELCHER, KIENITZ, PELLERIN, SIGGIA, ZÝKA.

### 2. General Remarks

This Commission at the 1967 Conference in Prague was given a new direction in view of the already signed contract with CE. The collaboration with CE comprises primarily the recommendation of analytical methods for testing and control of different preservatives, antioxidants, colours, *etc.*, used in foodstuffs or as foodstuff-additives. The work was initiated by the Secretary General together with Prof. R. TRUHAUT and a contract was signed. As a first step the Commission was deliberately kept small without electing a Secretary, until one could see clearly the direction which the work would take. Some vague proposals were made on the occasion of a joint meeting between the Coordinating Committee and the Chairman of this Commission in Prague on 3rd September, 1967. Later, from the Secretary General the Chairman received about 10 methods on different materials without clear instructions except the wish to approve these as official IUPAC recommendations. The first reading showed us that the methods were generally, from the standpoint of analytical chemistry, far removed from being standard methods. Therefore, Prof. BELCHER and the Chairman met in Vienna on 12-14th December, 1967, and evolved a scheme for handling this matter. At Eastbourne in March 1968 this scheme was approved by the Coordinating Committee. The methods were then redrafted and sent via the Secretary General to the Members of our Commission. Only a few observations were offered. It came to our attention that these drafts had not been sent to Dr. A. C. FRAZER (Chairman of the Food Section) before March 1969. On 10th April, 1969, Dr. FRAZER called a meeting in London with the purpose of clarifying the situation. Those present at that meeting were: Dr. FRAZER, Dr. MORF, Prof. TRUHAUT, Dr. H. EGAN, Dr. M. WILLIAMS, and the Chairman of Commission V.1. This meeting rescheduled the material for CE. The work had to be completed by 30th May (because of the urgent needs of the Secretary General) so that it was divided amongst Prof. MALISSA, Dr. EGAN, and Prof. TRUHAUT — Dr. MORF. As far as we know the work from every side finished at the right time. However, the methods under consideration could not be designated as official IUPAC recommendations because there was no discussion with the Members of this Commission and no approval by the Analytical Chemistry Division Committee. Therefore, they had to be submitted for comment at Cortina.

The work and the mode of operation showed us clearly that there is surely a need of such a Commission but the task is far from clear and needs some new directions given by the Division President. If the work with CE becomes more heavy then Commission V.1 must be larger and the cooperation with the Food Section closer.

### 3. Meetings in Cortina

The Commission met three times in Cortina and discussed the above methods at length. Before these discussions could take place a lot of work had to be done and we are thankful also to the Members of the Food Section concerned with it.



The situation is as follows:

A. Approval for further handling through the proper channels was given to the following methods:

- (a) No. 20—Nachweis von Calcium in Milchsaeure, Na- und K-Lactat.
- (b) No. 21—Nachweis von Chloriden in Milchsaeure, Na- und K-Lactat.
- (c) No. 22—Nachweis von Hexacyanoferrat(II) in Milchsaeure, Na- und K-Lactat.
- (d) No. 23—Nachweis von reduzierenden Substanzen in Milchsaeure, Na- und K-Lactat.
- (e) No. 24—Bestimmung der Sulfatasche in Milchsaeure, Na- und K-Lactat.
- (f) No. 25—Bestimmung von Eisen in Milchsaeure, Na-, K- und Ca-Lactat.

B. The following methods are, after small changes and redrafting, to be regarded as tentative: Nos. 2, 4, 5, 6, 7, 8, 9, 10, 11, 15, and 16.

C. Three methods are to be checked by laboratory tests:

- (a) No. 1—Dosage de l'arsenic dans glycerine a usage industriel (Prof. PELLERIN).
- (b) No. 3—Determination of Isatin-5-sulphonic Acid (Prof. PELLERIN).
- (c) No. 19—Nachweis von Ba in Calciumlactat (Prof. BELCHER).

D. Methods Nos. 17 and 18, concerning the Identification of Oxalic Acid and Ba in Lactic Acid and Lactates, are rejected and alternatives should be found.

#### **4. Recommendation**

To ensure a closer liaison with the Food Section, Prof. PELLERIN had agreed to serve as the Coordinator from our side and it is to be hoped that a similar step will be taken by the Food Section.

On 4th July the new Chairman of the Food Section, Dr. EGAN, and Prof. MALISSA had a discussion on this matter and agreed to a closer cooperation.

#### **5. Membership**

It was agreed in Prague in 1967 that Prof. MALISSA would work only for 2 years as the Chairman of the Commission. Because of the fact that the future work of the Commission will increase more and more, the Commission membership needed to be filled up to the statutory number. It asked, therefore, for approval of the following new Members: Dr. A. HULANICKI (Poland), Mr. F. J. REIDINGER (USA), Dr. B. WEIBULL (Sweden) as Titular Members; Dr. J. BARTOS (France), Prof. L. SOMMER (Czechoslovakia), Prof. H. WEISZ (Germany) as Associate Members.

Prof. ZÝKA was appointed as Secretary.

### **Joint Meeting of Commission V.1 and Section VI.1**

1. The meeting took place on 1st July. Those present were: MALISSA (in the chair), BELCHER, PELLERIN, SIGGIA, ZÝKA (Commission V.1) and BUSHILL, EGAN, COLLINGS, MARCUSE, REITH, TRUHAUT (Section VI.1). Prof. P. W. WEST was in attendance.

2. The meeting discussed the general interest in the Food Section in methods of analysis and agreed that, where these methods were received from outside IUPAC, joint evaluation between the Commission and the Section was desirable. Members of the Section welcomed the general co-operation of the Commission on all matters of analysis. Where methods of analysis originated within the Section, copies of these would be sent to the Commission as a matter of courtesy.

3. The meeting discussed in particular the arrangements for evaluating methods of analysis proposed under the present contract between IUPAC and CE. Dissatisfaction was expressed with the earlier arrangements for the selection and presentation of these methods but the scheme drawn up at the meeting held in London on 10th April, 1969, which had subsequently been implemented in relation to the 28 methods currently under consideration, had proved basically satisfactory other than that the time available for evaluation had been inadequate. There was, however, also need for a systematic method for the selection of methods to be evaluated. The present meeting agreed that further consideration should be given to the formation of a small Joint Working Group of the Commission and the Section to progress any future arrangements under this contract.

4. At a further joint meeting held in Cortina on 4th July between Prof. BELCHER, Dr. EGAN, and Prof. MALISSA it was agreed that a Joint Working Group of the Commission and the Section should be established which would meet on the occasion of IUPAC Conferences (and, if necessary, at other convenient times), both to progress IUPAC-CE arrangements and for general liaison. Prof. MALISSA announced that Prof. PELLERIN had been nominated by the Commission and Dr. EGAN announced that Dr. MARCUSE, Dr. OSER, and himself had been nominated by the Section. It was agreed that these four Members, together with Prof. BELCHER, should constitute the Joint Working Group and that Prof. PELLERIN and Dr. MARCUSE would act as Correspondents for the Commission and the Section, respectively.

5. Dr. EGAN said that the 'Eastbourne' format for the presentation of methods of food analysis was satisfactory, but drew attention to an alternative format published by the International Organization for Standardization in ISO TC/34 (Agricultural Food Produce) Recommendation No. R 71. Prof. BELCHER agreed to examine this document. It was also agreed that the Food Section would, in the normal way, be responsible for the initial selection of methods of food analysis for evaluation. Dr. EGAN said that, apart from expert opinion of the Commission on Analytical Reactions and Reagents on the validity of the methods then elaborated, there was particular need for advice on the use of analytical terms such as accuracy, precision, sensitivity, selectivity, reproducibility, repeatability, *etc.*, and also on the corresponding terms in other languages.

## COMMISSION V.2: MICROCHEMICAL TECHNIQUES AND TRACE ANALYSIS

### I. Meetings

The Commission met on 1st and 2nd July. Those present were: SCHÖNIGER, LÉVY, O. KOCH, W. KOCH, VEČEŘA (Titular Members); MALISSA (in part), CHENG (in part) (Associate Members).

### 2. Reports

(a) *Study on the Accuracy and Precision of Methods for the Determination of Carbon and Hydrogen in Organic Compounds* (Project Leader: VEČEŘA). The report would be published at the end of 1969 or the beginning of 1970, according to information from the Division Secretary.

(b) *Study on the Sources of Errors in Elementary Organic Microanalysis* (Project Leader: LÉVY). The draft of the report (288 pages) was approved in Cortina by the Commission. It would now be submitted to the Division Committee for approval, after having been reproduced in the Secretariat. The Commission asked the Division Committee to examine this report as fast as possible, so that it might be given to the publisher towards the end of 1969. It had to be considered that this study had been delayed considerably due to several difficulties (see *Comptes Rendus XXIV Conference*) and that any longer delay would create the risk of making the report out of date.

### 3. Current projects

#### (a) *Elementary Microchemical Analysis*

- (i) *Study on the Accuracy and Precision of the Determination of Fluorine in Organic Compounds* (Project Leader: MACDONALD). It had been already stated (see Status Report, March 1969) that the first attempt to carry out this study had been a failure due to technical reasons. In the absence of Dr. MACDONALD the Commission decided to ask her to communicate to its Members the results previously obtained from the microanalysts who cooperated in this study. From another viewpoint, the Commission thought it would be necessary to make an enquiry in order to estimate the number of microanalysts willing to cooperate in the second part of this study where a given combustion procedure and a specific titration were involved. Estimated date of completion: 1971.
- (ii) *Study on the Accuracy and Precision of the Determination of Nitrogen (according to Dumas in Organic Compounds)* (Project Leader: VEČEŘA). Prof. VEČEŘA had received 54 answers to the 350 questionnaires he sent out. He proposed to start the second part of the study and to send samples for analysis to the microanalysts willing to cooperate. The Commission found the number of 54 answers to be satisfactory and agreed with Prof. VEČEŘA's proposals. He summed up his remarks, concerning the answers to the questionnaire and his proposals, in a short report. Estimated date of completion: 1970.
- (iii) *Study on the Accuracy and Precision of Carbon and Hydrogen Determinations in Organic Compounds Containing Heteroelements* (Project Leader: GEL'MAN). Because of the late arrival in Cortina of Dr. GEL'MAN (3rd July) the preliminary orientation which resulted from the answers she received to a questionnaire (see Status Report, March 1969) would be circulated within the Commission. Estimated date of completion: 1971.



- (iv) *Study on the Accuracy and Precision of the Determination of Metals in Organic Compounds excluding Simple Residue Procedures* (Project Leader: KÖRBL). Because it had been impossible to contact the Project Leader during the last 2 years, the following decision was made. The new Titular Member Dr. G. INGRAM would be asked to take over as Project Leader. Estimated date of completion: 1971.

(b) *Trace Analysis*

- (i) *Study on Mass Absorption Coefficients Used in Electron Beam Microanalysis* (Project Leader: MALISSA). A preliminary draft report from Prof. MALISSA had been approved by the Commission. After a meeting of the participants in this study in Vienna in October 1969 it would be decided to what extent the preliminary report should be published in the *Information Bulletin*. This study should finally lead to the publication of a book. Participants in this study: Prof. MALISSA, Prof. W. KOCH, and Dr. HEINRICH. Estimated date of completion: 1971.
- (ii) *Study on the Purification of Chemicals Used for Micro and Trace Analysis* (Project Leader: O. G. KOCH). Because the project leader Prof. FLASCHKA had terminated his IUPAC activities, Dr. KOCH, who was already participating in this project, took over as Project Leader. He gave the Commission a short written report on the status of this project, concerning the purification of reagents used for analysis. Because analysts from some important countries (e.g., France, USSR) had not been consulted the Commission suggested that Dr. KOCH should complete these enquiries. Estimated date of completion: 1970.

#### 4. Proposed New Projects

(a) *Microchemical Analysis*

*The Expression of Error in Organic Analysis* (Project Leader: PELLA). It is a standard practice in organic elementary microanalysis to give absolute limits of errors ( $\pm 0.3\%$ ). Although this might have been justified with classical milligram analysis it had no special significance any longer. The Commission proposed to work out recommendations for a more scientific expression of errors on the basis of *Recommendation for the Presentation of the Results of Chemical Analysis* (*Information Bulletin* No. 26, p. 39). Estimated date of completion: 1971.

(b) *Trace Analysis*. The Commission welcomed the proposal from the USSR National Committee, transmitted by the Division President, to study the Unification of Analytical Techniques for the Determination of Minor Amounts of Impurities in High-grade Chemicals. It had been decided to start a study on:

- (i) *Trace Analysis Applicable to Determination of Minor Amounts of Impurities in High-grade Chemicals* (Proposed Project Leader: PINTA). A preliminary enquiry had to be made of analysts, institutes, and laboratories working in the field of trace analysis and willing to co-operate. If suitable personnel for this study could be found, a proposal for initiating the project would be submitted to the Division Committee before the next Bureau Meeting (1970).

In a second step test materials would be sent to selected laboratories which would be asked to have them analysed by given analytical procedures. After evaluation of the results, recommendations would be proposed and published (Project Leader: O. G. KOCH). Estimated date for completion of the enquiry: 1970.

- (ii) *Study on Trace Impurities in Oxygen and Helium* (Project Leader: CHENG). Procedures for the determination and elimination of impurities in both gases were to be recommended. Estimated date of completion: 1971.

### **5. Special Comments**

The Commission requested permission to meet during the *VIth International Symposium on Microchemistry* in Graz 1970. At that time some current and new projects would be discussed. No subvention was required.

## COMMISSION V.3: ANALYTICAL NOMENCLATURE

### 1. Meetings

The Commission met during the period 1st-4th July. Those present were: BELCHER, T. S. WEST, BAYER, IRVING, SAMUELSON, SANDELL (Titular Members); AMBROSE (Associate Member).

### 2. Previous Meetings

The minutes of the meetings held in Prague on 30th-31st August, 1967, and in London on 20th September, 1968, were confirmed. Arising from the minutes the Secretary reported that the Bureau had confirmed the appointment of Dr. A. J. B. ROBERTSON in place of Dr. BIEMANN because the latter had declined to accept Associate Membership.

### 3. Ion Exchange

Prof. SAMUELSON reported that the ion-exchange report was now complete following approval by the *ad hoc* Working Group. It would be published in the *Information Bulletin*. The Commission expressed the desire that such information of a tentative nature might be published in journals such as *Anal. Chem.*, *Analyst*, *Z. für Anal. Chem.*, etc.

### 4. Chromatography

The report on nomenclature for chromatography was discussed extensively. Dr. AMBROSE agreed to draft another report to be discussed at a special meeting of the Working Group at Tübingen on 25th October (AMBROSE, BAYER, IRVING, SAMUELSON). Financial support for Dr. AMBROSE and Prof. IRVING was to be requested from the Division; Profs. SAMUELSON and BAYER would already be in Tübingen. The finalized Tübingen version of the report would be duly circulated according to an agreed schedule.

### 5. Mechanization and Automation

The report on mechanization and automation was considered at length. General observations from Prof. KAISER were discussed but in the absence of detailed comments the Commission did not consider it necessary to make changes to the final version to be considered by Council on 5th and 7th July.

### 6. Trivial Names

Prof. IRVING's compilation on trivial names was discussed and warmly approved by the Commission. Because Members had not yet had sufficient time to consider the report it was suggested that comments should be sent to Prof. IRVING by 31st December, 1969. Meanwhile, copies were to be passed to the Inter-Divisional Committee on Nomenclature and Symbols, and to the American Chemical Society Committee dealing with a similar project.

### 7. Scales of Working

The document on scales of working drawn up by Prof. SANDELL's Working Group was discussed in detail, and it was agreed to circulate it for further comment by interested parties, e.g., Microchemistry Group of the Society for Analytical Chemistry (SAC), Metropolitan Microchemical Society, before further action by the Working Group.



## 8. Standard Substances

The report produced by Dr. STEPHEN was received. Lack of progress on this project was largely due to the feeling of the Working Group that rapid and definitive progress could be more readily accomplished after the SAC Analytical Methods Committee Sub-Group had completed further reports on standard substances. These should soon be ready. It was suggested that Prof. ALIMARIN and Prof. LASTOVSKY be approached to check the addresses of Russian Members because, in some instances, there had been lack of communication.

## 9. Contamination Phenomena

Little progress had also been made on this project. The Secretary agreed to ask Dr. BERG once more to initiate definitions of terms already agreed. It was also suggested that Prof. FISCHER and Dr. ZETTLER might formalize definitions independently.

## 10. Mass Spectrometry

A list of terms requiring definition in the project on *Nomenclature for Mass Spectrometry* was received from Dr. ROBERTSON. The Commission expressed the wish that Dr. ROBERTSON should proceed with definition of these terms. It was suggested that Dr. ROBERTSON might attend the Tübingen meeting to discuss the project with Profs. SAMUELSON and BAYER.

## 11. Other Projects

Reports on the progress of the newly initiated projects (London 1968) of *Selectivity Index*; *Presentation of Analytical Methods for Publication*; *Terminology for Normality, Molarity, and Formality* were received.

## 12. Future Projects

With regard to future work, the Commission had 9 active projects on hand, only 2 of which were in advanced stages. A new project on *Kinetic Methods in Analytical Chemistry* was suggested. Prof. IRVING would undertake leadership of this project. It was noted that Dr. A. TOWNSHEND and Dr. G. SVEHLA might be approached to help with this project. Another possible project was concerned with *Nomenclature on Molecular Absorption and Fluorescence Emission Spectroscopy*. Before such a project was undertaken it would be necessary to ascertain the activities of Commission V.4 in this area.

## 13. Chairman 1969-1973

Because of other commitments placed upon him by the Division, Prof. BELCHER announced his retirement as Chairman. The Commission expressed its regret at his departure and unanimously recommended that Prof. IRVING be appointed as the new Chairman.

## **COMMISSION V.4: SPECTROCHEMICAL AND OTHER OPTICAL PROCEDURES FOR ANALYSES**

### **1. Meetings**

The Commission met on 30th June, 1st and 2nd July. Those present were: KAISER, FASSEL, ALKEMADE, BILLS, KVALHEIM, PLŠKO (Titular Members); MENZIES, RUBEŠKA (Associate Members).

### **2. Reports**

A few minor corrections were made to the nomenclature document entitled *Nomenclature, Symbols, Units, and Their Usage in Spectrochemical Analysis —I*. This report was now ready for publication as a tentative recommendation. The report had been officially approved by Commission I.1.

### **3. Nomenclature, Symbols, Units, and Their Usage in Flame Atomic Absorption, Emission, and Fluorescence Spectroscopy**

The purpose, content, and a general outline of a document on this subject were discussed in detail during two sessions of the Commission. Prof. ALKEMADE has been appointed Chairman of a Task Group to expedite completion of this project. Other members of the Task Group were: BILLS, MENZIES, FASSEL, RUBEŠKA, MASSMANN, HERRMANN, KAISER, AMOS, WINEFORDNER, and ROBINSON. Because of the urgency in completing this document, the Commission was planning to meet in 1970 to discuss and approve the tentative report for publication.

### **4. Task Group on Nomenclature in X-Ray Fluorescence Spectroscopy and Electron Microprobe Analysis**

The Task Group, consisting of BIRKS as Chairman and DEVRIES and BILLS as Members, circulated a list of terms and symbols at an informal meeting of the Commission held at the *XVth Colloquium Spectroscopicum Internationale* in Madrid in May 1969. The estimated completion date for this document is 1971.

### **5. Task Group on Description and Classification of Light Sources**

A Task Group, consisting of SCRIBNER (Chairman), FASSEL, and KAISER, had formulated a general plan. Discussions were held at Madrid in May and in a 1-day informal session in Washington in June. The estimated completion date of this document is 1971.

### **6. Task Group on Terms, Concepts, and Definitions leading to a Rigorous Determination of Detection Limits**

A document was being prepared by KAISER. The completion date is September 1969. The last open questions were cleared in Cortina and at an informal meeting at Athens, Georgia, in June 1969.

### **7. Minimal Detectable Concentrations**

This project would be completed after the conclusion of Item 6 above.

### **8. Extraordinary Meeting**

A request to hold an extraordinary session of the Commission in central Europe in 1970 would be submitted. This session was required to complete the task discussed under Item 3 above.



## COMMISSION V.5: ELECTROANALYTICAL CHEMISTRY

### I. Meetings

The Commission met on 1st, 2nd and 4th July. The following members were present at all meetings: KOLTHOFF, ZUMAN, CHARLOT, KEMULA, MEITES, PERRIN, TANAKA (Titular Members); BISHOP, TRÉMILLON (Associate Members); FUJINAGA (National Representative).

### 2. Minutes of Prague Meetings (1967)

These were approved.

### 3. (a) Symposium on Non-Aqueous Electrochemistry

This would be held under the joint sponsorship of Commissions I.3 and V.5 in Paris on 8-10th July, 1970. Prof. CHARLOT serves as President, and Dr. J. BADOZ had accepted responsibility to organize the symposium as Executive President. The programme would consist of Prof. CHARLOT's Introduction, Prof. KOLTHOFF's General Inaugural Lecture, plenary lectures by BARD (US, on organic electrochemistry), CAUQUIS (France, on organic electrochemistry), by LAGOWSKI (US, on solvation), by PARKER (Australia, on equilibria in dipolar aprotic solvents), STREHLOW (Germany, on solvation in non-aqueous media), and TRÉMILLON (France, electrochemistry in molten salts). Each lecture would be presented in 45 min, and 15 min will be reserved for discussion. It was planned also to have 13-14 general lectures (30 min+15 min for discussion). The following names had been suggested for these lectures: BADOZ, ADAMS, TANAKA, LAITINEN, GERISCHER, FUJINAGA, KOZLOWSKI, JUILLARD, SAWYER, COETZEE, COUTEAU, BATES, and DAVIES. Members of Commission I.3 would send their suggestions to Dr. BADOZ. The selection of topics and speakers was entrusted to the Organizing Committee. Only the Australian lecturer would get 50% of his travel expenses reimbursed; the other plenary lecturers would receive subsistence for 3 days. Commission I.3 had requested from IUPAC \$1,000 for the Organizing Committee in Paris and this request was supported by Commission V.5.

### (b) Expenses for Meeting Paris 1970

Funds for travel and subsistence expenses of the Chairman and Secretary of Commission V.5 for a meeting in Paris in July 1970 with Commission I.3 were requested. (The entire Commission I.3 had been allowed travel and subsistence expenses for its meeting in July 1970 in Paris.) A joint meeting with the Chairman and Secretary of Commission I.3 was highly desirable for a continued discussion of subjects of interest to both Commissions I.3 and V.5 to secure cooperation on certain projects and to avoid overlap of activities.

### 4. Old Business

(a) *Polarographic Data*. A. A. VLČEK (Czechoslovakia) was preparing critically selected data of half-wave potentials of inorganic substances and would make this compilation available to Commission V.5. Dr. ZUMAN was preparing a statistically evaluated list of half-wave potentials of benzenoid substances based on linear free energy treatment. Prof. MEITES and Dr. ZUMAN were engaged in an effort to ensure cooperation between centres in various countries on the publication of bibliographies. Data cards covering the period 1966-68 had been prepared by Prof. FUJINAGA, who would prepare a critically selected list of half-wave potentials.

(b) *Purification of Solvents.* A report by L. M. MUKHERJEE on purification of pyridine had been received. It would be commented on by Prof. TRÉMILLON and prepared in the final form by Prof. KOLTHOFF before December 1969. It would then be submitted for publication. A report on purification of propylene carbonate by T. FUJINAGA and K. IZUTSU was submitted by Prof. FUJINAGA. This report would be revised using the report of L. KNECHT as a model of organization. It would be resubmitted in the final form before July 1970. The report by L. KNECHT was approved for publication at the meeting in Prague; it would be submitted to the Division Committee. The Secretary would receive information on the report by REDDY from Prof. KOLTHOFF who would contact the author. The literature on solvent purity was available in Prof. CHARLOT's laboratory. Authors were sought for the following solvents: DMF, TMF, acetic acid, nitromethane, sulfolene, and acetone. Profs. TRÉMILLON and KOLTHOFF were willing to review new reports. Eventual publication of all individual reports in the form of a monograph was recommended.

(c) *Purification and Purity of Reagents.* Z. GALUS would submit before December 1969 a report on purification of hydrochloric acid and ammonia as supporting electrolytes in stripping analysis for electro determination of traces of metals and a list of other reagents to be studied. Use of the electro-active carbon tetrachloride in dithizone extractions was considered questionable. Possibility of controlled potential electrolysis in reagent purification was discussed. Mr. BISHOP would submit before October 1969 a report on the purification of sulphuric acid from organic impurities. Commission V.2 had projects on purification and tests for purity and would cooperate with V.5 on such subjects. Prof. TRÉMILLON was nominated representative in an interdisciplinary Commission on purity. Mr. FENNELL would contact Chairmen of other Commissions which had projects dealing with purity and would request them to appoint a representative to the interdisciplinary Commission.

(d) *Electrochemical Data in Non-Aqueous Solvents.* A table of dissociation constants of acids and salts in pyridine (L. M. MUKHERJEE) was submitted and reviewed. Collection of pK values in non-aqueous solvents would be continued and a report would be submitted in 2 years for some 3-4 solvents. A preliminary compilation of inorganic half-wave potentials in dimethylformamide, prepared by J. F. COETZEE, was presented. It would be revised and submitted to the Commission for approval. It was suggested that a critically prepared compilation of ion mobility in organic solvents should be transferred to Commission I.3.

(e) *Effect of Pretreatment of Solid Electrodes on Characteristics of Electrode Reactions.* A preliminary report prepared by N. TANAKA with cooperation by a group of Japanese chemists was presented and discussed. The project was being continued with the cooperation of Mr. BISHOP. Cooperation of B. TRÉMILLON, G. CHARLOT, J. BADOZ, S. BRUCKENSTEIN, and H. A. LAITINEN would be solicited. More detailed information on the method of measurement of cathodic and anodic limits should be incorporated, as well as details on preparation of certain electrodes, e.g., carbon paste. It was recommended to restrict the report to the analytically used electrodes.

## 5. Old and New Business

(a) *The Classification of Nomenclature of Electroanalytical Methods.* The 1959 Report by P. DELAHAY, G. CHARLOT, and H. A. LAITINEN would be revised, updated, and extended to include definitions of d.c. and a.c. voltammetry and

other modern techniques by L. MEITES in cooperation with H. W. NÜRNBERG (to be contacted by Prof. MEITES) and Dr. ZUMAN. Cooperation with H. A. LAITINEN was being solicited. The first draft of definitions would be prepared before 1st January, 1970.

(b) Commission V.5 requested the Division Committee to consider the delay in publication of reports. Reports that have not been sent to the printer within 1 year after submission should be returned to the author for updating.

(c) *pK Values of Organic Bases*. The Commission recommended that Dr. PERRIN revise and update his pK compilation of organic bases. The manuscript would be ready before July 1971.

(d) *Cooperation with Commission I.3*

(i) The programme of the jointly sponsored *Symposium on Non-Aqueous Electrochemistry* had been discussed.

(ii) Commission V.5 was opposed to TEXTS I and II on *Sign Convention Concerning Galvanic Cells and Electrodes* submitted to Commission I.3.

(iii) It was requested that Members of Commission V.5 be kept informed on the progress of the project on electrochemical kinetics of Commission I.3.

(iv) It was suggested to publish jointly the programmes of Commission I.3 and V.5 in journals.

(v) The Group dealing with electrochemical nomenclature in Commission V.5 would restrict itself to electroanalytical techniques; other terminology would be dealt with by Commission I.3.

(vi) A sample of the compilation of electrochemical data prepared by G. MILAZZO would be circulated to all Members of Commission V.5. Comments and criticism were requested by Commission I.3.

(vii) Copies of the preliminary report by N. TANAKA on *Pretreatment of Solid Electrodes* would be sent to Members of Commission I.3 with a request for comments and criticism (see also minutes of Joint Meetings of Chairmen and Secretaries of Commissions I.3 and V.5: p. 85).

(e) *Oxidation-Reduction Potentials*. The report *Constantes sélectionnées. Potentiels d'oxydo-reduction des corps minéraux en solution aqueuse* by G. CHARLOT, A. COLLUMEAU, and J. C. MARCHON was approved. Six copies would be sent by G. CHARLOT to the Division Secretary within 3 weeks for approval by the Division Committee. Three copies would be sent to Commission I.3, after the 6 copies were returned by Mr. FENNELL.

(f) *The Use of Coulometry for Standardization of Solutions*. The objective was to reappraise the Laitinen Report. Particularly the following three matters would be considered:

(i) to establish whether coulometric determinations could be carried out with a precision and accuracy commensurate with the best assays of primary chemical standards and the precision of the reference atomic mass standard, silver;

(ii) to develop a working theory of coulometric processes which could be tested experimentally and used to predict conditions required to yield a high current efficiency;

(iii) to canvass the opinion of practising electroanalytical chemists as to whether the conclusions of the Laitinen report still stand or should be amended.

(g) *Other Items*. R. C. KAPOOR would be requested to present a report on the status of electroanalytical chemistry in India.

The Commission would seek information on election procedures in other Commissions with the aim of unification.



The Commission proposed to the Division Committee that the number of years of Associate Membership before the *first* election to Titular Membership not be included into the 8-year period.

## 6. Elections

Prof. KOLTHOFF was re-elected Chairman with his provision that he would not stay for more than 2 years. He was ready to stay in order to define clearly cooperation with Commission I.3. In place of Titular Members Profs. TANAKA and CHARLOT, whose terms expired, and Prof. KEMULA, who resigned, the following were elected: Prof. B. TRÉMILLON, Dr. Z. GALUS, and Mr. E. BISHOP—all unanimously. Profs. KEMULA, CHARLOT, and TANAKA, and Dr. J. K. TAYLOR were suggested to act as National Representatives. The following Associate Members were elected for the next 2 years: Prof. BRUCKENSTEIN, Prof. COETZEE, and Dr. H. W. NÜRNBERG (re-elected); Prof. T. FUJINAGA, Prof. R. C. KAPOOR, Prof. H. A. LAITINEN, and Prof. A. A. VLČEK.

## COMMISSION V.6: EQUILIBRIUM DATA

### 1. Meetings

The Commission met on 1st and 2nd July. Those present were: MARCUS, ROSSOTTI, ANDEREGG, BECK, LEUSSING, ROGERS, YAMASAKI (Titular Members); HUME, SILLÉN (Associate Members).

### 2. Nomenclature of Separation Methods

Members of the Commission met the *ad hoc* Committee on Nomenclature of Analytical Separation Processes and Members of Commission V.3 to discuss terminology in ion exchange and chromatography. Recommendations concerning various distribution ratios were agreed.

### 3. Critical Surveys of Stability Constants

Prof. BECK was appointed project leader, and agreed to circulate a paper on the principles of critical evaluation together with an updated version of his survey of cyanide complexes, which was first discussed at the XXIVth IUPAC Conference. Progress made by Prof. YATSIMIRSKII and Dr. VASIL'EV on their survey of bismuth halides was uncertain. Dr. ANDEREGG agreed to circulate a survey of EDTA and other aminopolycarboxylate complexes in April 1970. Members of the Commission were urged to initiate other surveys for groups of ligands or metal ions.

### 4. Distribution Equilibria

Specimen tabulations for some phosphoric acid extractants were discussed and drafts for a further group of phosphorus ligands, together with a general introduction to the tables would be circulated by Dr. KERTES and Prof. MARCUS during the coming winter. Work on chelating extractants by Profs. DYRSSEN and FREISER was less far advanced and it was decided to invite Dr. STARÝ to assist in this part of the work. It was clear that the project could not be completed in 2 years and it might be most practicable to publish separate reports on groups of extractants.

### 5. Standard Ionic Media

Comparison of equilibrium data was difficult because of the wide variation in choice of ionic medium. It was resolved to invite Dr. BIEDERMANN to investigate the feasibility of recommending standard ionic media and of giving criteria for a particular choice.

### 6. Tables of Stability Constants

Prof. SILLÉN reported that the supplement to the 2nd edition of the *Tables of Stability Constants* prepared by himself and Prof. MARTELL should be ready to go to press in August. The supplement updates the 2nd edition to 1968 and also included stability constants inadvertently omitted from the 1st and 2nd editions. The possibility of differentiating Brønsted (or mixed) constants for acids from activity and concentration quotients was discussed, and a plea made for a more durable binding than those used for the previous volumes. Prof. YAMASAKI tabled a list of stability constants published in Japanese during the period May 1967-December 1968. Prof. SILLÉN expressed his willingness to organize the inorganic part of a further supplement to appear in 4 or 5 years time, but did not know whether Prof. MARTELL was able to continue with the organic part. Problems of information retrieval were

discussed and Prof. LEUSSING agreed to investigate the possibility of assistance from Chemical Abstracts in the form of a code symbol on the abstracts of papers which contain, for example, equilibrium data.

### **7. Equilibria in Non-Aqueous Solvents**

A letter from Prof. MISUMI (Japan) concerning definitions and symbols for equilibrium constants obtained in non-aqueous and mixed solvent media was discussed. The approach indicated in the Commission's report on *Recommended Symbols for Equilibria* was considered to be more appropriate than a proliferation of superscripts and subscripts.

### **8. Selected Values of Stability Constants**

A tabulation of selected values of equilibrium constants (25°C and zero ionic strength) had been made by Prof. SILLÉN and Dr. HÖGFELDT and would be distributed to the Commission for checking. Comments should be sent to Prof. SILLÉN before 1st November, 1969.

### **9. Miscellaneous**

Possible future projects, suggested by Prof. ROGERS, on the effect of systematic structural changes in ligands on solution equilibria, and on equilibria in gas chromatography were considered.



## COMMISSION V.7: ANALYTICAL RADIOCHEMISTRY AND NUCLEAR MATERIALS

### 1. Meetings

The Commission met on 1st and 2nd July. The following were present: COOK, MEINKE, CRESPI, MINCZEWSKI, SMALES (Titular Members); HECHT, KOSTA (Associate Members).

### 2. Purity of Commercial Radioactively Labelled Preparations

The report of this enquiry had been approved by the Division Committee and was in the hands of the Secretariat for final processing for publication.

### 3. Publicity for Radioactive Methods in Analytical Chemistry

(a) The completed 108-page draft of the article *Radiochemistry in Analytical Chemistry* was discussed in Cortina. A few minor changes were suggested and a deadline of 1st September was set for final corrections. This would then permit the submission of the final manuscript to the Division Secretary by 1st October.

(b) A second very important area in urgent need of publicity regarding its present status was *Light Element Analysis by Radiochemical Methods*. An outline of an article would be prepared in the next 6 months and then a first draft of the article would be developed for consideration at the 1971 IUPAC Conference.

(c) A third very important area for which a current status report was urgently needed was *High Energy Photon Activation*. A schedule similar to (b) above would be followed.

### 4. Intercomparison of Analytical Methods

(a) The first efforts of the Commission in this area which were initiated four years ago involved the intercomparison of several different analytical methods for the determination of uranium in low-grade ores. The report for this work was now in final draft. One extensive set of comments on the report from a collaborating laboratory was considered at Cortina and would be resolved by 1st September. Thus the final report would be submitted to the Division Secretary by 1st October.

(b) The interest and experience in intercomparisons generated in the above effort had contributed to the plans for a characterization exchange sponsored by OECD. Although there was as yet no formal contact with IUPAC, one of the Commission members was Chairman of the OECD exchange and 3 others would be participating in the experimental procedures. In this exchange 5 very high purity, single crystal materials were to be characterized for trace elements and defects by more than 50 different laboratories using 8 different chemical and physical trace methods.

The members of the Commission plan to follow closely the progress of the OECD exchange and then to plan before the 1971 IUPAC Conference for possible additional exchanges to help improve the sensitivity and accuracy of various trace analytical methods. Such improvement was of particular importance in connection with the certification of the reference materials described below in Item 5.

## 5. Reference Materials for Activation Analysis

The summary of information on reference materials for activation analysis prepared by Division members for Cortina had shown the need in many fields for samples with certified trace analyses. Although the interests of the Commission were initially in radiochemical methods it soon became apparent that activation analysis was only one of a number of trace analytical methods which could use such materials. A number of high-purity materials of high homogeneity were now available in quantity. For each of these materials analytical values had been determined for a few trace elements but much more information could be determined by various trace methods.

The Commission proposed to encourage scientists in many areas of trace analysis to cooperate in developing information on additional elements in these materials. Periodically the Commission would summarize these values and publish recommended values in *Pure and Applied Chemistry*. At the same time a list of currently available reference materials would be compiled and submitted for publication.

## 6. Problems in Analysis of Nuclear Materials

The concept of *State of the Art* reports on subjects of analyses of nuclear materials had been agreed by the Commission members to be an important and useful contribution to the analytical literature. Such reports would summarize methods of analysis for principal, minor, and trace elements, together with limits of detection, accuracies, and precisions to be expected. The specimen draft on the analysis of beryllium oxide would be completed and two further subjects would be started—the analysis of uranium oxides and the analysis of graphite.

## 7. Source Materials for Radiochemistry

(a) At the request of the Sub-Committee on Radiochemistry of the US National Academy of Sciences–National Research Council attempts had been made to compile a companion edition to its *Source Materials for Radiochemistry*. The objective of this NAS-NRC volume was to provide a list of authoritative books, reviews, and articles of relatively wide scope. These references were, however, all in the English language and the objective of the companion would be to provide a similar list in languages other than English. While many references had been collected from correspondents the volume remained incomplete. A further consideration of the collection, brought up to date, would be made in the next year with a view to a final decision as to the form of publication.

(b) A new project proposed was to compile a list of authoritative reviews on radiochemistry in various languages, interpreting the subject matter in a relatively wide sense. Because nowadays it was difficult for a scientist to be aware of even a majority of reviews in a broad field such as radiochemistry, it was felt that a bibliography of reviews classified according to subject would be of great value.

## 8. National Regulations for Use of Radioisotopes

National regulations for the procurement and handling of the small amounts of radioactive material sufficient for many radioanalytical investigations varied enormously from country to country. It was felt that the development of radiochemistry was handicapped where regulations did not permit the easy procurement of such small quantities. The problem had been brought to

the attention of the International Atomic Energy Agency and it was believed that future consideration from that body would give sympathetic consideration for the point of view of the Commission.

### **9. Nomenclature**

Part I of a glossary of terms in radiochemistry (comprising 73 items) had been agreed upon and was now ready after final typing for circulation to other Commissions concerned with nomenclature. Part II of this work would be undertaken during the coming 2 years.

### **10. Reagents**

The letter prepared for manufacturers of chemical reagents urging them to label any reagent prepared from material of abnormal isotopic abundance (particularly lithium, uranium, and boron) with at least a warning that the isotopic abundance *may not be normal* had been approved by the Division Committee, the IUPAC Executive Committee, and the Chairman of the Joint Commission on Applied Radioactivity, and was being circulated by the Secretariat.

A second circular letter intended for scientists working in analytical radiochemistry enquiring whether they found reagents of sufficient purity for their work had been approved by the Division Committee and was being circulated by the Secretariat to a list of scientists provided by the Commission.

### **11. Conventions for Flux Monitoring and Definition of Sensitivity in Radiochemical Methods**

The Commission saw the need for establishing conventions in a number of areas of radiochemistry. There is at present a 'Texas' convention rather generally accepted for monitoring the flux for 14-Mev neutrons obtained from small generators which were widely used for activation analysis. For several other irradiation facilities (e.g., high energy  $\gamma$ -machines and charged particle accelerators) no such convention existed at present and comparison of results from different machines was difficult. Because interest in this field was rapidly expanding, the early establishment of such conventions was essential for proper coordination of results. Similar problems existed in the determination of the sensitivity of detection of elements by radiochemical methods. Before the 1971 IUPAC Conference, Commission Members would develop a draft of the above conventions.



# OPEN MEETING OF THE ANALYTICAL CHEMISTRY DIVISION

3rd July 1969

## I. President's Opening Remarks

The Division President, Prof. P. W. WEST, expressed his appreciation of the work of the Division and of the Division Committee. He thanked those who were retiring from the Committee and welcomed those who had just been elected; he introduced Prof. KEMULA as the new President and expressed his best wishes for a successful term of office.

In reviewing his term as President, Prof. WEST paid particular tribute to Prof. MALISSA for his help as Vice-President during the first 2 years and for taking over the Division's work on the CE Programme. He was also pleased to acknowledge the help and advice of Prof. BELCHER. The sudden death of Dr. DEGENS had thrown a severe strain on the administration of the Division but, with the continued support of the Secretary General, Dr. MORF, the co-operation of the present Division Secretary and, lately, the establishment of the Secretariat at Oxford, the Division was now running well.

Prof. WEST referred to the valuable cooperation with Prof. TRUHAUT, Applied Chemistry Division, during the work on the CE Programme. He hoped that cooperation between the two Divisions would grow and thought that the most active growth of IUPAC would take place in the two Divisions as more help was requested from the Union by other organizations.

## 2. Division Committee 1969-71

The Secretary formally announced the elections of Profs. FISCHER (Germany), FREISER (USA), and TANAKA (Japan) to the Division Committee, 1969-73.

## 3. Publications

The Secretary announced the latest information he had on the publication of reports finalized by the Division at or after the Prague Conference. He also referred to the announcement of the Division's work which had been published in several analytical journals.

The main discussion was, however, concerned with the length and complexity of the procedure for publication of reports from Commissions, especially nomenclature reports, and the question of whether the circulation of *Pure and Applied Chemistry* was wide enough to ensure that the world's chemists were aware of the work of IUPAC. On the latter point, a strong plea was put in that publication of compilations of data and of nomenclature rules should be allowed in other journals.

The Secretary said that he thought there was little chance that publication in journals other than *Pure and Applied Chemistry* would be allowed except in special cases, e.g., where a first edition had been published before the journal started. He suggested, however, that a request for alterations in IUPAC rules for approval for publication of reports could be initiated or reinforced by a proposal passed by the Division which the President could put before the Bureau. The Secretary read out a draft proposal and the following resolution was proposed by Prof. ROGERS, seconded by Dr. MEINKE, and carried:

That the Secretary's proposal be adopted in principle but that a Working Group be empowered to finalize the wording without changing the sense.

Profs. KAISER and T. S. WEST and the Secretary were asked to finalize the wording, which is reproduced in *Appendix*.

#### **4. International Laboratory for Analytical Chemistry (ILACH)**

Prof. MALISSA said that his experiences with the CE work had shown the desirability of having some proper organization available which could arrange for the checking of analytical methods. An *ad hoc* Committee had been doing some exploratory work and had produced a short report which was read to the meeting. The report recommended the setting up of a Working Group on analytical quality control to examine the problem and obtain details on how it might be solved.

After considerable discussion, the following resolution was proposed by Dr. MEINKE, seconded by Prof. ROGERS, and carried:

That the recommendations of the *ad hoc* ILACH Committee be accepted; that a Working Group be set up by the Analytical Chemistry Division to examine the problem of analytical quality control and that limited funds should be made available by IUPAC.

#### **5. Revised Division Rules**

The Secretary explained that he was trying to update the rules, compiled by Dr. DEGENS in 1962, in a way that would give the maximum of help to Members of the Division. He expressed his gratitude to the many Members of the Division who had commented on the draft and explained that the Division Rules must be in accordance with the IUPAC Statutes and By-laws and be approved by Council.

The Secretary read out the proposals of the Division Committee regarding the status of Division Secretary and the replacement of Members of the Division Committee who did not complete their term of office.

Dr. ZUMAN said, in respect of By-law 4.1303, that Commission V.5 would like to propose that Associate Membership before Titular Membership should not count in the 8 consecutive years membership. He also asked that a further distribution of the Statutes and By-laws should be arranged if copies were available.

#### **6. Any Other Business**

(a) Prof. KEMULA thanked Prof. P. W. WEST for the work that he had done, during his period of office as Division President, for the advancement of the activities of the Division. He was glad Prof. WEST was remaining for another 2 years on the Division Committee and would thus be able to offer his help and advice. Prof. KEMULA then thanked his colleagues in the Division for his election to the Presidency. He knew he could depend on the Division to give him all the support he would need in order to continue the work his predecessors had started.

(b) Prof. HUME referred to the *ad hoc* Committee on Nomenclature of Analytical Separation Processes and stated that there was still apparently a need for the group to remain in existence. He distributed 2 reports produced by the Committee.

(c) Prof. T. S. WEST asked whether at future Conferences, it would be possible for the Chairmen and Secretaries of Commissions to meet, before the Commissions started work, so that questions of mutual interest could be coordinated.

## Appendix

The Analytical Chemistry Division requests permission of the Bureau:

1. To increase the Membership of the Division Committee to 11 Members, the Division Secretary being a non-voting Member, to take effect as from the elections for the 1971 Division Committee.

2. To bring into effect immediately the following passage proposed for the Rules of the Division:

'In the event of the resignation or death of a Committee Member more than one year before the expiry of his term of office, the Division Committee is empowered to make a temporary appointment tenable until a normal election for the relevant zone has taken place.'

3. To set up a Working Group to examine the problem of analytical quality control and requests the provision of limited funds from IUPAC for this Group.

The Division requests the Bureau to consider the following proposals for the publication of nomenclature reports:

1. After approval by the Division Committee, the report should be published in the *Information Bulletin* or in a special publication dealing with tentative recommendations.

2. A period of 4 months should be specified for the receipt of comments.

3. Comments should be sent to the relevant Commission Secretary.

4. (a) If no adverse comments are received, the Division President should ask the Bureau for permission to publish in *Pure and Applied Chemistry*.

(b) If adverse comments are received, the report should

(i) be considered by the Commission.

(ii) If the comments are rejected by the Commission or lead to a revised report, both the comments and the report (new or old) should be screened by a specially constituted Supervisory Committee drawn from within IUPAC.

(iii) The Supervisory Committee should be set up by the IUPAC Executive Committee with the advice of the Division Presidents.

(iv) The function of the Supervisory Committee should be:

(a) to ensure that all received comments have been duly considered;

(b) to ensure that all international regulations on symbols and units (e.g., ISO, Conférence Internationale de Poids et Mesures, etc., as well as IUPAC and IUPAP) have been observed. Obvious scientific or linguistic errors should be corrected.

(v) With this safeguard—which should be given in writing and signed by the Chairman of the Supervisory Committee and the Chairman of the relevant Commission—the document in its approved form should proceed directly to the Bureau for *rapid* publication.

(vi) At the next meeting of Council, the Bureau shall report to Council its action on recommending the report for publication and ask for approval of such action.



# APPLIED CHEMISTRY DIVISION COMMITTEE

30th June 1970

*Present:* Dr. W. GALLAY (in the chair), Prof. R. TRUHAUT, Dr. I. E. PUDDINGTON, Dr. R. W. CAIRNS, Dr. K. HOSHINO, Dr. W. G. STOLL (Titular Members); Prof. H. SUOMALAINEN, Prof. H. A. BOEKENOOGEN, Dr. H. HURTIG, Mr. P. H. FINK-JENSEN, Dr. S. FREYSCHUSS.

*In attendance:* Dr. R. MORF, Mr. H. K. RAASCHOU-NIELSON, Mr. H. J. VOS.

## 1. Opening Remarks

Dr. GALLAY welcomed the delegates and paid tribute to the excellent contributions to IUPAC of Dr. A. C. FRAZER. His untimely death was noted with great regret.

## 2. Statutes

A brief review and interpretation of IUPAC Statutes having a bearing on Division activities was made. In particular the following points were stressed:

- (a) Obtaining Bureau approval before soliciting funds from outside sources.
- (b) The possibility of joint activities with other Divisions of IUPAC and with other organizations.
- (c) Committee membership rules.

## 3. Committee Membership

(a) Dr. GALLAY stressed the need for industrial participation in IUPAC Units. There was general agreement that the balance between industrial, academic, and government types required constant review, particularly in the Applied Chemistry Division.

(b) Dr. GALLAY referred to the necessity of having nominations for Committee membership available before the meeting on 3rd July.

## 4. Secretariat in Oxford

The Chairman suggested that as much use as possible be made of the excellent service provided by the new Secretariat. It was noted also that copies of all correspondence dealing with IUPAC activities should go to the Secretariat in the interest of correlating and expediting Division work.

## 5. Finances

Dr. GALLAY stressed the need to operate in as economical a manner as possible and referred to the existence of the Division President's contingency fund.

## 6. Symposia

The rules and procedure governing symposia and also President KONDRATIEV's message concerning them were reviewed. The points stressed were: the requirement for high scientific quality and literary style of manuscripts and presentations, no financial aid from IUPAC in general in a IUPAC Congress/Conference Year, the clearing of themes with the Bureau, the mechanism of obtaining financial aid, credit for IUPAC sponsorship, and the first refusal for publication from *Pure and Applied Chemistry*.

Discussion brought out that rigidity of IUPAC rules on symposia sometimes gave hardship to organizers. Dr. MORF explained that the restrictions imposed by a contract with Butterworth's may be partially responsible, but it was felt that the problem was amenable to negotiated solution.

## **7. Publications**

A problem seemed to arise with material such as Section progress reports and some specialized symposia proceedings where the subject matter was not suitable for publication in or did not reach the interested people if it were to appear in either *Pure and Applied Chemistry* or the *Information Bulletin*. A compromise by which a brief summary prepared by the active participants would appear in the *Information Bulletin* and a more complete report by the same authors would be published in an interested journal, seemed agreeable to all and should be acceptable to Butterworths.

## **8. Company Associates Plan**

Dr. MORF reviewed IUPAC history, pointing out that the organization had been founded by industrialists but these founders had gradually been replaced by more academic types. To restore the balance Lord TONN had made the proposal that industrial companies could, by paying one or more units (\$250 or multiples of this amount), become Company Associate members. Hopefully this would lead to closer industrial ties and eventually allow more industrial chemists to be appointed to IUPAC Units where their special knowledge would be valuable. The National Adhering Organizations had been responsible for the presentation of this scheme. USA and Japan had been particularly successful with 94 and 21 units, respectively; there was now a total membership of more than 150 units. Analytical standards and procedures available through IUPAC had been the most attractive feature of the arrangement to industry.

## **9. ICSU**

Dr. GALLAY referred to the activity of ICSU on the subject of human environment. Two meetings sponsored by ICSU had been held. The most recent one in Stockholm was described by Prof. TRUHAUT who attended the meeting and would report later to the Bureau. The subjects covered at the meeting included agricultural, chemical, effluent, thermal and acoustical pollution, soil erosion, and over population. Dr. CAIRNS expressed the view that IUPAC should use a more aggressive approach in associating itself with this work and Dr. GALLAY would raise the subject with the Bureau.

## **10. Any Other Business**

In reply to a question by Prof. SUOMALAINEN, Dr. MORF explained that Division Open Meetings were held to inform delegates, who might not otherwise have the opportunity of learning about the activities in the various Divisions. Future plans as well as current activities would thus be suitable agenda subjects.

*3rd July 1969*

*Present:* in addition to those present on 30th June, all Sections except VI.7 were represented.

## **1. New Members**

The new Members nominated by the Sections and Commissions were elected unanimously en bloc.

## 2. Joint Problems and Projects

On the invitation of the Chairman, the Section representatives commented as follows:-

*Food*—Dr. EGAN: Analytical methods were frequently of general application and items of interest would be circulated beyond the Section (that related to food and to toxic substances analysis).

*Organic Coatings*—Mr. FINK-JENSEN

*Oils and Fats*—Dr. HEINERTH

*Water, Sewage, and Industrial Wastes*—Dr. FREYSCHUSS

*Toxicology*—Prof. TRUHAUT

} All indicated  
they had  
no problems.

*Pesticides*—Dr. HURTIG: The Section and its Commissions had already established liaison with other interested Sections and with the Analytical Chemistry Division.

*Fermentation*—Dr. LANGLYKKE: It was indicated that liaison with Sir RONALD NYHOLM or his successor would be established on the teaching of bio-engineering—and with the Food Section on work on single cell proteins.

General guidance from the Analytical Chemistry Division on nomenclature was considered highly desirable by several of the Sections. (Subsequent conversation with Dr. EGAN suggested that this information was being sought already by a direct approach.)

## 3. Elections

After reading several Statutes, it was noted by Dr. GALLAY that the Applied Chemistry Division had no By-laws. Election of new Officers, therefore, proceeded without prior notice.

*Vice-President.* On a motion by Dr. STOLL, seconded by Prof. TRUHAUT, Dr. R. W. CAIRNS was unanimously elected as Vice-President of the Division.

After some discussion, it was decided that Dr. GALLAY should approach the Bureau for permission to elect 2 additional Titular Members. The subject would be discussed with Dr. REES first. The importance of selecting active Members, if possible from industry, was stressed strongly.

## 4. Human Environment

The question was again raised of stronger IUPAC representation in the ICSU programme on human environment. Prof. WIDMARK and Prof. TRUHAUT, invited expert Observers to the Stockholm meeting on this subject, would make a report to the Bureau. Dr. GALLAY would make a strong plea to the Bureau for aggressive action on the part of IUPAC.

Dr. GALLAY presented a letter from the Pesticides Section recommending that he be made an IUPAC Representative on SCOPE. The Pesticides Section also proposed the establishment of an *ad hoc* Committee to give advice to the IUPAC Representative on SCOPE. Dr. GALLAY would take these proposals to the Bureau.

## 5. Symposia

Dr. GALLAY would speak to the Bureau about the establishment of a Steering Committee to organize the proposed symposium on *Chemical Contributions to Present and Future Food World Supplies*, a subject favoured by the Applied Chemistry Division Committee at its meeting in Montreal on 1st-2nd October, 1968. The suggestion that this symposium be combined with the *IIIrd*



*International Congress on Food Science and Technology (SOS/70)* (SOS = Science of Survival) in USA was not favoured. An IUPAC-sponsored symposium for 1973 with emphasis on the Chemistry of Food received support from Pesticides, Fermentation, Oils and Fats, and Food Sections. Dr. EGAN would propose a list of names for possible Committee Members.

#### **6. Inter-Divisional Committee on Nomenclature and Symbols**

Prof. S. J. PIRT was unanimously endorsed as the Applied Chemistry Division Representative.

#### **7. Any Other Business**

Mr. FINK-JENSEN raised a particular problem in publications. IUPAC sponsorship was sought for a series of monographs with the possible title *Progress in Surface Coatings*. This proposal had been strongly endorsed by the Organic Coatings Section, and would appear to be financially self-liquidating because sales would probably run to 2,000 volumes. As this appeared to be a part of the general publications policy problem, Dr. GALLAY would review the whole subject with the Bureau.

## SECTION VI.1: FOOD

1. The Section met on 2nd, 3rd and 4th July, Commissions VI.1.1 and VI.1.2 also convening during this period. Tribute was paid to the memory of the Section Chairman, Dr. A. C. FRAZER, who died suddenly on 14th June.
2. The Section made arrangements for the updating and rapid publication of the survey completed earlier of methods of analysis for the determination of certain additives in food.
3. The structure of the Section and its Commissions was discussed in detail and required revision. The present membership of the Food Additives and Contaminants Commission was virtually identical with the Section membership, whereas there was very little overlap of the Trace Substances Commission and Food Section memberships. At the same time, the titles of the two Commissions were insufficiently distinctive. This situation also meant that the heavy programme of the Section and its two Commissions was at present carried by a total membership which was limited in number to that normally accorded to a Section and a single Commission. Full attention would be paid to these difficulties in the next 2 years.
4. The Section considered jointly with Commission V.1 (Analytical Reactions and Reagents) the methods of analysis of food additives elaborated by the Coordinating Committee in pursuance of the 1968 contract between IUPAC and CE. Joint arrangements had been made with the Commission for the rapid consideration of such methods of analysis on future occasions.
5. At the request of the Netherlands Nutritional Council, advice on the nomenclature of vitamins had been given in conjunction with the Joint IUPAC-IUB Commission on Biochemical Nomenclature
6. The Section supported a proposal that IUPAC should sponsor an international meeting on *Chemical Contributions to Present and Future World Food Supplies* and, having regard to arrangements already announced by the International Committee on Food Science and Technology regarding the *IIIrd International Congress of Food Science and Technology* to be held 10-14th August, 1970, recommended 1973 for the date of the IUPAC meeting.
7. The programmes of the Food Additives and Contaminants Commission, the Trace Substances Commission, and of the Mycotoxins Sub-Commission and the Smoke Constituents Sub-Commission were reviewed. It was agreed that further meetings of the Section, its Commissions and Sub-Commissions should be held in the Netherlands, 14-16th September, 1970.

### Commission VI.1.1: Trace Substances

The volume and importance of the work of the current two Sub-Commissions had reached a point where it was felt that two full Commissions should be formed in the near future, namely, a Commission on Smoke Constituents and a Commission on Mycotoxins.

#### Sub-Commission VI.1.1.1: Mycotoxins

1. Stage 3 of the collaborative exercise in aflatoxin analysis had been completed and a provisional method published in the *Information Bulletin*. Problems of stability of standards delayed operations for a year. These had now been resolved in a collaborative exercise. The Sub-Commission confirmed its confidence in the methodology, which was inherently versatile, with capability for modification for use in different countries. The Sub-Commission considered that it had at least 2 years' work in hand.

2. The future programme of the Sub-Commission would include:

- (a) The appraisal of a rapid method for aflatoxin analysis (WALKING *et al.*, *J. Assoc. Off. Anal. Chem.* **45**, 880 (1968)) on the basis of published evidence and on published American collaborative data.
- (b) A collaborative analytical programme directed initially towards the simultaneous analysis of aflatoxin and other mycotoxins.
- (c) The establishment of lines of guidance for *clean-up*.
- (d) Consideration of the need for collaborative analysis for aflatoxin contamination of dried roots and certain other foods (other than groundnuts) in international trade.
- (e) The study of new work on the analytical methodology of nephrotoxin.
- (f) The further investigation of analysis of milk products for aflatoxin M.

#### **Sub-Commission VI.1.1.2: Smoke Constituents**

1. Following up the extended collaborative assay on the benzo(a)pyrene in 1968, samples of fish containing 0, 4, and 10 ppb of benzo(a)pyrene were sent to several laboratories for further analysis using any method desired; the results were acceptable. Some difficulty was reported with the Florisil, pointing to the need for better control of the reagents, and not all the reagents were available internationally.

2. The question of extending the sensitivity of the method to 2 ppb was discussed but the consensus of the group was that it was not necessary at this time to try for the lower level of hydrocarbon. Dr. BOGOVSKI (International Agency for Research on Cancer, WHO) stated that possible co-carcinogens or other potentiators can influence even trace amounts of the carcinogen.

3. The question of the advisability or need for a multi-component collaborative assay was also discussed, and it was noted that an International Agency for Research on Cancer report stated that an assay for polynuclear hydrocarbons should include 6 compounds: benzo(a)pyrene, dibenz(a,h)anthracene, and dibenz(a,h)acridine as carcinogens, and the non-carcinogens benzo(g,h,i)-perylene, pyrene, and coronene. The latter were included because they could be mistaken for the carcinogens. It was noted that a multi-component assay had been proposed to the Association of Official Analytical Chemists (AOAC) in USA and it was agreed to approach AOAC requesting joint collaboration with IUPAC in this work.

4. The Sub-Commission considered aspects of a report on the meeting of the Working Group on Food, IARC, with respect to the analysis of polynuclear aromatic hydrocarbons. There was a question as to whether a single extract could be used for the examination of two or more different groups of carcinogens (*i.e.*, polynuclear hydrocarbons, nitrosamines, or aflatoxins). It was felt that no single solvent would quantitatively remove all classes; separate samples should therefore be extracted with appropriate solvent. With respect to the immediate examination of extracts in areas of the world where analytical laboratory facilities were not available, IARC indicated that no information was available on the storage stability of the polynuclear hydrocarbons. The Sub-Commission was unaware of any problem of stability and indicated literature references to stability of these compounds. On the question of a comparison between the IUPAC analytical procedure for trace polynuclear compounds and the method recently mentioned by Dr. GRIMMER, further details of the latter were requested for review and evaluation.

5. The Sub-Commission reaffirmed that top priority should be given to work involving the assay of polynuclear hydrocarbons and the study of nitrosamines should be referred to the Food Section for proper assignment.



### **Commission VI.1.2: Food Additives and Contaminants**

1. The Commission considered a compilation of specifications of 7 solvents used in the food industry, selected by FAO/WHO and prepared by the Commission. This information had been prepared with the object of recommending specifications for minimum standards for each of the solvents. A draft report was prepared and it was recommended that this should be submitted both to FAO/WHO and to industry (producers and users of solvents) for comment. When such comments had been received, within a period of 6-9 months, the Commission would, if necessary, introduce amendments to the specifications and, if desired by FAO/WHO, a study of additional solvents be undertaken.
2. In addition to the above-mentioned 7 solvents for special study, a list of specifications for some 40 other solvents had been prepared from literature available. This list would serve as a basis for any further study.
3. A preliminary survey of the literature on the detection and determination of solvent residues in food had also been prepared. It was proposed that this study be continued, particularly as the draft report for FAO/WHO above disclosed the need for information on the subject. It was also proposed to ask industry for any information available on the detection and determination of residues of solvents in food.
4. It was recommended that the following items should remain on the programme of the Commission:
  - (a) in conjunction with the Food Section, to review methods of analysis for the purity of food additives as required under the terms of the current IUPAC-CE contract;
  - (b) to review further food additives for which methods of analysis on food are needed in the interests of international trade.

## **SECTION VI.2: FERMENTATION INDUSTRIES**

### **1. Meetings**

The Section met on 1st and 2nd July. The following were present: SUOMALAINEN, LANGLYKKE, PARISI, FIECHTER, HOGERHEIDE, PIRT (Titular Members); BUNKER, LIGHT (Associate Members). Apologies had been received for non-attendance from LUNDIN, MALÉK, PEPLER (Associate Members). Dr. WUTZEL (Institute for Cereal Chemistry) was in attendance. After a brief introduction, the Chairman said some words in memory of Prof. DREWS (Associate Member) who had died recently.

### **2. IVth International Fermentation Symposium (Kyoto, 1972)**

Trends to follow and requests that would have to be made in order to assure more significance to the sponsorship by IUPAC and to obtain the best results from a meeting of so great importance were discussed. Dr. HOGERHEIDE would get in touch with the Organizing Committee during his visit to Japan in August.

### **3. International Standards for Ethanol Content of Alcohols and Spirits**

Note was taken of the publication of the paper, prepared at the Research Laboratory of the Finnish State Alcohol Monopoly, in *Pure and Applied Chemistry*. The widest circulation would be given to this paper by sending Prof. SUOMALAINEN names and addresses of all organizations that are interested in the matter.

### **4. Methods for Dry Baker's Yeast Evaluation**

The progress report for publication in *Pure and Applied Chemistry*, prepared by the Secretary, was authorized and it was agreed to collect a series of experimental data on the influence of factors until now considered of minor importance in fermentation power determination.

### **5. World Survey on Fermentation Industries**

Dr. LANGLYKKE was collecting material with great difficulty and he hoped that he would be able to give a more complete report at the next meeting.

### **6. Standards for Fodder Yeast from Hydrocarbons**

Dr. HOGERHEIDE spoke about the present position of the Working Group. The task was to find out analytical methods and to prepare specifications that in this case also had to consider possible toxicity. The Working Group was requested to continue its very interesting and fruitful enquiry.

### **7. Bioengineering Teaching**

The subject was debated and finally it was agreed to investigate the possibility of organizing an open seminar about it. This seminar could be organized by Prof. PIRT in England or by Dr. FIECHTER in Switzerland in 1970. Final decisions would be taken by correspondence.

### **8. Agreements with Water, Sewage, and Industrial Wastes Section**

The Officers of the Fermentation Section were charged to get in touch with

those of the Water, Sewage, and Industrial Wastes Section in order to study the possibility of common work. Initial contacts had subsequently been made and the opportunities for collective work would now be examined.

#### **9. Next Meeting**

This would be in June 1970, the exact date and the place to be decided and communicated by correspondence.



## SECTION VI.3: OILS AND FATS

1. The meeting of the Section was held under the Chairmanship of Prof. BOEKENOOGEN on 2nd July. The total number of participants, including Observers, amounted to 30.

2. In his opening address as well as in his Section report Prof. BOEKENOOGEN commemorated the passing away of Mr. W. V. LEE on 11th March and of Mr. G. WOLFF on 13th April of this year, two former Members of great value. They always participated with great enthusiasm and devotion in the work of the Section. Mr. WOLFF was one of the founders of the International Committee for the Study of Oils and Fats, which became the Oils and Fats Section of IUPAC in 1947; he was Chairman of the Section from 1961 to 1965.

3. As to the composition of the Section, the following nominations were approved by the participants:

Dr. H. A. BRÜGGER (Switzerland) to succeed Dr. J. KLEINERT;

Dr. J. A. JAKUBOWSKI (Poland) to replace Dr. H. GRYNBERG;

Dr. Ö. LEVIN (Sweden) to succeed Dr. G. WODE;

Mr. A. T. MØLLER (Denmark) to replace Mr. J. T. ERRBOE;

Ing. J. B. ROOS (Netherlands) in place of Prof. H. A. BOEKENOOGEN;

Dr. A. D. SCOTT (UK) to succeed the late Mr. W. V. LEE;

Dr. J. C. VAN DER WEEL (Netherlands) to succeed Dr. F. HOEKE.

With the exception of the Secretary, all Titular Members were replaced. The assembly unanimously agreed with the nomination of Dr. E. HEINERTH (Germany) as the new Chairman, of Ing. M. MALENICKÝ (Czechoslovakia) as the new Vice-Chairman, and of Dr. P. B. CZEDIK-EYSENBERG (Austria), Dr. N. D. EMBREE (USA), Prof. G. JACINI (Italy), Dr. G. LOEW (Italy), and Dr. K. A. WILLIAMS (UK) as the other new Titular Members.

In order to bring the composition of the Section into agreement with the Statutes and By-laws of IUPAC a number of Associate Members were nominated for the coming period of 4 years: Mr. T. W. BREADEN (Ireland), Dr. J. A. CORNELIUS (UK), Prof. E. L. DELVAUX (Belgium), Mr. B. GULL-BRANDSON (Sweden), Dr. H. HADORN (Switzerland), Prof. J. MARTINEZ-MORENO (Spain), Prof. M. NAUDET (France), Mr. A. PETERSEN (Denmark), Prof. A. RUTKOWSKI (Poland), and Mr. J. P. WOLFF (France).

New Zealand joined the Oils and Fats Section, Mr. S. G. BROOKER of Abels Ltd., Auckland, becoming the National Representative.

4. The participants discussed the results of the investigations carried out in accordance with the Work Programme for 1968-1969: determination of mono-, di- and tri- glycerides by column chromatography; determination of chlorinated pesticides in oils and fats by gas chromatography and thin-layer chromatography; determination of elaidic acid by thin-layer chromatography in combination with gas chromatography. The first one was adopted as a standardized method with some modifications to be introduced in the text, while it was decided to continue the study of the other two methods, based on modified texts, with new samples as part of the Work Programme for 1969-1970. As to this Programme it was also agreed that a comparison should be made between the determination of elaidic acid in question, the determination of this acid by direct gas chromatographic separation on a capillary tube and the determination of trans fatty acids by means of infrared spectrophotometry.

Concerning the three bleaching tests for crude palm oil, the texts of which were distributed in May 1969, it was decided not to investigate them but to

create a Sub-Committee, consisting of 5 Members, which should consider the methods in question (to which has to be added also the AOCS methods) and their possibilities.

5. As to the next Meeting of the Oils and Fats Section, the Swedish delegation invited the Members to come to its country for the Réunions-1970, which in principle could be organized on 3rd and 4th September.

## SECTION VI.4: TOXICOLOGY AND INDUSTRIAL HYGIENE

1. The Section met on 1st and 2nd July. Those present were: TRUHAUT, BOUDÈNE, FREDERICK, LUXON, METRICO, MONKMAN, PILZ, VASAK (Titular Members); GAGE, PIETRULLA, WEST (Associate Members). Madame BUSH-TUEVA (USSR) had declined an invitation to participate in the Section's activities, even as an Associate Member, by reason of her work as a consultant with ILO and WHO.

2. After unanimous approval of the minutes of the previous meeting in Prague, 1967, the Section was informed of the following publication, by Butterworths, of methods for the 6 materials listed below:

- Mercury in air
- Trichlorethylene in urine
- Sulphur dioxide in air
- Acetone in air
- Mercury in urine
- Arsenic in urine

Five other methods were nearly ready for publication, as follows:

- Metabolites of trichlorethylene in urine
- Lead in urine
- Carboxyhaemoglobin in blood
- Benzene in blood
- Hydrochloric acid in air

The measurement, in air, of the following toxic materials was discussed in the light of work done by Members of the Section:

- Methyl bromide—adopted
- Sulphuric acid mist—adopted
- Cadmium—adopted
- Lead fumes—adopted
- Iron oxide fumes—adopted
- Antimony—adopted
- Ozone—to be submitted to further study
- Phosphine—to be submitted to further study
- Hydrofluoric acid—to be submitted to further study
- Mercaptans—to be submitted to further study

The methods adopted above would be put in proper format for publication.

3. The important question of the use of indicator tubes, for a screening or alarm method, was discussed and some general guide lines for their manufacture were established and would be published.

4. For the first time, the Section had considered the study of measurement of toxic compounds present in industrial solvents and discussed, in particular, the measurement of benzene in complex solvent mixtures. Finally, methods for measurement of the following were discussed, as present in biological materials:

- Phenol in urine—a new procedure would be circulated for cooperative test
- Cholinesterase activity in whole blood
- Cholinesterase activity in red cells
- Cholinesterase activity in plasma

The 3 methods for cholinesterase activity were adopted in principle, but the Section decided to subject them to a supplementary laboratory investigation before submitting them for publication. The same procedure was to be followed for the measurement of lead in urine by polarography.



5. A discussion took place on the work in progress relating to the standardization of methods suitable for use in connection with the control of air pollution. The following contaminants were discussed:

- Sulphur dioxide
- Sulphuric acid mist
- Hydrogen sulphide
- Mercaptans
- Nitrogen oxides
- Carbon monoxide
- Ozone
- Selenium
- Lead and other elements

6. The Chairman presented information on the setting up of a new Working Group on the analysis of potential carcinogens present in the atmosphere and submitted for approval the composition of this Group. It would work with the International Union against Cancer (UICC) and the International Agency for Research on Cancer (IARC) attached to WHO. The first studies were to be on polycyclic aromatic hydrocarbons, nitrosamines, asbestos, mineral oils, and various mineral compounds.

7. The Section decided unanimously to request the Bureau and Council, as well as the Division Committee, for approval to organize a colloquium on the quantitative measurement of carcinogens in the environment. It was hoped that the Food Section would also be interested in such a colloquium which could thus become a symposium in which other organizations could participate, *e.g.*, UICC and IARC.

8. The problem of establishment of methods of analysis of sensitivity applicable to threshold limit values had been examined once more and some recent information was presented by the Chairman.

9. After recapitulating the various cooperative activities associated with international organizations, the Chairman proposed to the Section as part of its future programme, the study of methods for the measurement of the following contaminants:

- |                                      |  |
|--------------------------------------|--|
| (a) <i>In the air of work places</i> | Chlorinated hydrocarbons (alarm)<br>Isocyanates, used in plastic manufacture<br>Nitroglycol<br>Hydrazine, used in welding<br>Organomercurials<br>Nickel carbonyl<br>Crystalline silica dust (quartz)<br>Asbestos |
| (b) <i>In urine</i>                  | Mercury by UV absorption<br>Vanadium in blood<br>Delta amino levulinic acid  |
| (c) <i>In urban air</i>              | Sulphur dioxide<br>Mineral dusts<br>Nitrogen oxides  |

To these methods were to be added those submitted to further studies (see above) which were the object of the study of the Working Group on Carcinogens.

10. The Section decided to hold its next meeting on the occasion of the IUPAC Conference in 1971.

## **SECTION VI.5: PESTICIDES**

### **1. Meetings**

The Section met on 1st and 6th July. The following Titular Members were present: HURTIG, RESNICK, ABBOTT, COOK, FREHSE, GALLEY, HILL, SUTHERLAND, WIDMARK.

### **2. Minutes of 1968 Meeting**

These were adopted.

### **3. Titular Membership expiring in 1969**

- (a) Mr. COOK (USA) and Dr. RESNICK (Israel) were re-elected for a further period of 4 years, with Dr. RESNICK to serve as Secretary of the Section.
- (b) With regard to Dr. HURTIG (Canada) and Dr. GALLEY (UK) the Section decided to request special permission from the Bureau for their re-election for a further period of 4 years, Dr. HURTIG to continue as Chairman of the Section and Dr. GALLEY as Chairman of Commission VI.5.2.

### **4. New Titular Member**

The Section decided to nominate Dr. K. FUKUNAGA (Japan) to fill the vacancy in the Titular Membership of the Section. When approved by the Division and the Bureau, the Section decided to assign Dr. FUKUNAGA to Commission VI.5.1.

### **5. Policy of Work of Commissions VI.5.1 and VI.5.2— Relation to FAO/WHO and Codex Alimentarius Requirements**

- (a) The Section reviewed the policy of work of Commissions VI.5.1 and VI.5.2 to meet the growing requirements of FAO/WHO and the Codex Alimentarius Committee on Pesticide Residues in pesticide terminal residues and standardized analytical methods, and decided to stress the need of strengthening the work of the two Commissions. This would be done by assigning definite areas where new information is needed to Titular and Associate Members, who would act as *Research Coordinators* for soliciting the information and see to it that the work needed was actually done.
- (b) In this connection, the Section strongly urged that better liaison be established with FAO and WHO, especially by its having a full feed-back of information from the Joint FAO/WHO Meetings of Experts on Pesticide Residues. It was the unanimous opinion of the Section Membership that although a very useful summary of the requirements of the Joint FAO/WHO Meeting had been supplied by the Secretariat of FAO (FAOPINS Status Report) the considerations of the two IUPAC Commissions were often handicapped by delays in publication of the monographs from the preceeding Joint Meeting, which contained the technical justifications for further research, together with the appropriate references. The Secretary of the Section was asked to bring this fact to the attention of WHO and FAO, and to urge that higher priority be given to the production and availability in time of future editions of these monographs.
- (c) On request by the Section, the President of the Applied Chemistry Division informed the Section of his decision to appoint its Chairman, Dr. HURTIG, as Spokesman of this Section to the Codex Alimentarius Committee

on Pesticide Residues. The Secretary would inform the Chairman of the Codex Committee on this matter.

## **6. ICSU Programmes on Human Environment**

The Section considered the United Nations projected efforts on *Human Environment*, the United Nations Conference to be held in Sweden in 1972, and ICSU's role in these projects under SCOPE..

The Section decided to draw the Division's attention to the following points:

(a) It was hoped that IUPAC would be invited to join SCOPE.

(b) The Section recommended strongly to the Division that the Bureau ensured that IUPAC would indeed be invited to join SCOPE, and that an *ad hoc* Committee drawn from the various Sections of the Division be formed, to lend scientific advice and briefing to the designated IUPAC representative on SCOPE.

In view of the importance of this projected work to the Applied Chemistry Division of IUPAC, this Section recommended to the Division Committee to make a strong and emphatic request to the Bureau to designate the President of the Applied Chemistry Division as the IUPAC representative to SCOPE.

## **7. OECD Work on Pesticides Residues**

The Section noted that OECD had a programme on the Unintentional Contamination of the Environment by Pesticides, and that an OECD Meeting would be convened in Netherlands in September 1969 to discuss analytical problems connected with the said programme. The Section decided to request the Division to appoint Prof. WIDMARK as IUPAC representative to this OECD Meeting.

## **8. FAO/IAEA Joint Division's Work on Pesticide Residues**

By invitation, Dr. P. WINTERINGHAM reported on the activities and programmes of the FAO/IAEA Joint Division in the field of pesticide residues. This Joint Division drew a scheme to encourage researchers to make use of labelled techniques for solving pesticide residues problems, especially with regard to metabolism of pesticides and their terminal residues. The reports of work in this field, resulting from the Joint FAO/IAEA Programmes, would be made available to the Section and its Commissions. The Section also noted that it would have close contact with these FAO/IAEA projects through the FAO Pesticides Programmes.

## **9. Publication Policy—Progress Reports**

The Section discussed at length the problem of publication of progress report papers prepared by Commissions Members, on subjects assigned to them by the Commissions. The Section decided as follows:

(a) Each author should indicate in his progress report paper where he would eventually publish his paper.

(b) The Secretary of the Section would arrange with the Secretariat in Oxford for the reproduction of all progress reports, and ensure that these could be made available, by request, from the Secretariat.

(c) The Chairman of the Section would appoint a Titular Member as an Editor to produce a *Newsletter*, containing all the titles of the progress report papers submitted to date to the Section and its Commissions and an indication



where these papers, in their final form, would be published. This Newsletter would be circulated to all Titular and Associate Members, and Observers from international organizations connected with the Section's work.

## **10. International Pesticide Chemistry Congresses of IUPAC**

(a) *IInd Congress* (Israel, 1971). Drs. HURTIG and RESNICK reported on behalf of the Organizing Committee of this Congress on the progress made in the preparations, and outlined the draft scientific programme for the Congress. Numerous suggestions were made regarding the scientific programme to be brought to the attention of the Israeli National Organizing Committee. The Section also discussed the *IUPAC Symposium on the Chemistry of Terminal Pesticide Residues*, to be held in Tel-Aviv, Israel, in conjunction with the IInd Congress.

(b) *IIIrd Congress* (Finland, 1974). Dr. P. KOIVISTOINEN reported that the Finnish Government had agreed that Finland would be host for the IIIrd Congress, to be held there in August 1974. A draft budget had already been prepared and an Organizing Committee was now being nominated.

## **11. Date and place of Next Meeting of Section and Commissions**

(a) 1970. The Section decided to request permission of the Division and the Bureau to hold the 1970 meetings of the Section and Commissions VI.5.1 and VI.5.2 between 14th and 18th September, 1970, in the area of Ingleheim, Germany, immediately following the IUPAC-sponsored *Symposium on the Chemistry of Pesticides under Metabolic and Environmental Conditions* (Bonn, 8-11th September, 1970).

(b) 1971. The Section noted that its 1971 meeting and those of its Commissions were to be held in USA within the framework of the XXVIth IUPAC Conference.

## **12. FAO and WHO**

At the end of the meeting, Dr. P. WINTERINGHAM thanked the Section on behalf of the Director-General of FAO, and stressed the fact that the Section was actually considered the scientific arm of FAO with regard to pesticides and their residues. The same feelings were also expressed by Dr. BERTEAU on behalf of WHO.

## **COMMISSION VI.5.1: TERMINAL PESTICIDE RESIDUES**

1. The Commission met on 1st, 2nd and 5th July. Those present were: HURTIG, HILL, COOK, GALLEY, SUTHERLAND (Titular Members); KENAGA, KORTE, POLEN, PORTER (Associate Members). Apologies for non-attendance were received from MOORE and SPENCER (Associate Members).

2. Members and visitors to the Fourth Meeting of the Commission were welcomed by the Chairman who explained the work of the Commission, stressing that the requirements specified jointly by FAO/WHO were used as the source of work for the Commission and cited the results obtained by Dr. POLEN in organizing laboratories in 8 countries to study terminal residues of chlordane.

3. The Chairman referred to the minutes of the Third Meeting held on 8-9th October, 1968, which, together with Appendices, had previously been circulated with minor corrections which were indicated; these were agreed.

4. Arising from the minutes of the Third Meeting, the Chairman referred to the following matters:

(a) The Report of the Biological Half-life Working Party (Appendix I) was presented by Dr. SUTHERLAND, who emphasized that confidence levels can be defined on harvested crops on a country by country basis and that advice must be given to growers as to when their crops can be harvested or shipped in order to contend with Codex tolerances. Following a lively discussion of the concept of *half-life*, the responsibility for advising growers, and revision of the report, it was agreed that the Summary Report should be considered a brief progress report and that the Working Party would draft an extended discussion of the concept of *half-life* for inclusion in the publication of the proceedings.

(b) The Secretary reported that summaries of the proceedings of the 1968 meetings had been published in *J. Assoc. Off. Anal. Chem.* **52**, 299 (1969); and that the full proceedings of the 1968 meetings had been published in *IUPAC Information Bulletin* No. 34, pp. 35-42.

(c) The FAO Status Report-1969 was considered by the Commission. The distinction between the terms *Required* and *Desired* as used in the Report was discussed and defined. Dr. WINTERINGHAM stressed that a specific date was attached to *Required* information which was needed in order to change a temporary tolerance to a permanent tolerance. The Commission agreed on the desirability of also having the full FAO/WHO Monograph available to Members before annual meetings. Arising from the requirements of the Report as summarized in the Agenda the Chairman delegated additional working assignments to appropriate members of the Commission.

## 5. Lindane

Very little new work was reported on terminal residues of lindane. The Commission received a report on work in progress on the metabolism of lindane-<sup>14</sup>C in wheat-seedlings, white cabbage, spinach, and carrots. After three days germination of the wheat-seedlings on an aqueous culture medium containing 207 ppm of lindane-<sup>14</sup>C about half of the radioactivity detected was due to metabolites of unknown structures which were more hydrophilic than lindane. Comparison of results with wheat-seed homogenates indicated that the metabolites were produced by the living plants and not by micro-organisms or environmental influences. Arising from the requirements of the FAO Status Report (Minute 4c) it was agreed that the Working Party would continue to collate and report results on terminal residues of lindane.

## 6. Cyclodiene Compounds

The report of the Working Party on Terminal Residues of Cyclodiene Insecticides was received (Appendix II). Considerable work was complete or in progress on metabolism in plants and animals, photochemical transformation, and biotransformation by micro-organisms of aldrin, dieldrin, photodieldrin, endrin, isodrin, heptachlor, heptachlor epoxide, chlordane,  $\gamma$ -chlordane, and endrin keto-isomer. The only new features were the findings that aldrin photoisomerized to a compound analogous to photodieldrin and that root-absorbed dieldrin was reduced to aldrin in stored cereal grains. Arising from the FAO Status Report it was agreed that the Commission would undertake to collate and report results on the chemical nature of terminal residues of

toxaphene in plants, animals, and their products as determined by modern analytical methods including the possible formation of photo-oxidation products.

### **7. Chlordane**

A report was received on work in progress on the terminal residues of chlordane (Appendix III). Reference was also made to work in progress on the plant metabolism of chlordane in which hydrophilic metabolites would be taken into consideration. It was noted that the terms alpha and gamma chlordane had now been changed to cis and trans. It was agreed that the Commission would continue to collate and report on progress in determining the terminal residues of chlordane.

### **8. Carbaryl and Other Carbamates**

A report was received on terminal residues of carbaryl and many other carbamates (Appendix IV). No new terminal residues of carbaryl had been reported due primarily to the difficulty in identifying aglycones. Recent work on other carbamates included studies of the metabolites of Furadan<sup>R</sup>, Temik<sup>R</sup>, Banlate<sup>R</sup>, Mobam<sup>R</sup>, Bux, and methomyl (Lannate). It was noted that the data on the latter two products represented a beneficial policy in the release of unpublished information from the files of US Food and Drug Administration (FDA) and a step forward in obtaining information for the Terminal Residues Commission. It was agreed that the Commission would continue to collate and report on terminal residues of carbaryl and other carbamates.

### **9. Dithiocarbamates**

The Commission received a report by Dr. SWISHER on unpublished work in progress on the metabolites or residues of Mancozeb in rats and plants using <sup>14</sup>C, <sup>35</sup>S, and tritium-labelled material. The same metabolites were found in plants and animals. Many compounds arising from acidic or basic hydrolysis *in vitro* were not found in either plants or animals. It was stressed that a method of analysis was needed which would pick up more than carbon disulfide. The Commission acknowledged the contribution of Dr. SWISHER who was invited to return next year for a further report.

### **10. Organophosphorus Compounds**

A report was received on recent work on the metabolites of malathion (Appendix V) in mammals which called attention to the fact that, of the two possible isomeric malathion monocarboxylic acids, it is the alpha monoacid that was exclusively produced *in vivo* and *in vitro*. Arising from the requirements of the FAO Status Report it was agreed that the Working Party would include in its reports information on terminal residues of azinphos-methyl, demeton-S-methyl sulphoxide, phosphamidon, coumaphos, and dioxathion. The report presented at the Third Meeting of the Commission by Dr. FREHSE had been published (E. MÖLLHOFF, *Pflanzenschutz-Nachrichten Bayer* 21, 401 (1968)).

### **II. Fumigants**

A report was received on the chemical nature of the terminal residues of fumigants (Appendix VI). It was pointed out that although the metabolites of ethylene oxide were well known no one had analyzed for all residues at the



same time. High residues of ethylene chlorohydrin were found in spices, herbs, seeds, and natural flavoring when they were fumigated with ethylene oxide. Ethylene bromohydrin was found in flour after ethylene oxide fumigation following a previous treatment with methyl bromide. Because of its rapid disappearance from foodstuffs there appeared to be no problem with methyl bromide residues. Mr. COOK reported that FDA had consistently found small amounts of chloroform along with carbon tetrachloride in grain treated with carbon tetrachloride. Dr. WINTERINGHAM called attention to the need for data on unchanged ethylene dibromide residues in fruits. Arising from the requirements of the FAO Status Report it was agreed to include future reports on the reaction products of ethylene oxide with food.

## **12. Rethrins and Synergists**

While there was no new completed work to report on the terminal residues of rethrins and synergists two projects were in progress—a study of the terminal residues of naturally degraded pyrethrins on grain and cabbage and studies on the metabolism of pyrethrins and synergists. These projects when finished would complete much of the information requested of the Commission.

## **13. Other Compounds**

(a) A report was received on the fate of organochlorine pesticides in vegetable oil processing (Appendix VII). The total evidence to date indicated that no significant levels of organochlorine compounds existed in process oils consumed by humans or in the seed cakes often used as animal feeds. However, byproducts such as soap stock or condensates from deodorization which were sometimes mixed in animal feeds may have organochlorine residues because the efficiency of removal by alkali-wash was low. In a communication to Dr. POLEN, Prof. DELVOE stated that *United States and European methods of oil processing were exactly the same with the exception of palm oil which was not deodorized as long because of its purity.*

(b) A report was received on the effects of washing, cooking, and other processing on residues of organochlorine pesticides (Appendix VIII). Results were highly variable depending on the pesticide involved, the food product studied, and the type and sequence of processing steps employed. In some instances virtually complete removal of residues was observed. The possibility of publishing this review in expanded form was mentioned and the paper on the influence of post-harvest factors on pesticide residues by H. STOBWASSER *et al.* [*Residue Reviews* 22, 45 (1968)] was noted.

(c) Arising from the requirements of the FAO Status Report it was agreed to collate and report on information on the nature of terminal residues of chlorobenzilate, chloropropylate, dicofol, and oxythioquinox.

## **14. Publication**

The Secretary was authorized to arrange for publication of the proceedings of the Commission by IUPAC and for a summary to be published in *J. Assoc. Offic. Anal. Chem.* The Secretary was further authorized to arrange for copies of unpublished Working Papers to be made available through the Secretariat.

## **15. Arrangements for Next Meeting**

It was announced that the next meeting of the Commission would be held at Ingelheim, Germany, on 14th to 18th September, 1970.

## APPENDIX I: Report of Biological Half-life Working Party

The real and apparent *disappearance* of pesticide residues from growing crops often generates a close mathematical approximation of a first-order decay curve and from this treatment of the data a pseudo biological half-life can be derived. While there may be a theoretical basis for this in a harvested crop, the phenomenon does not have a universal theoretical basis. However, although there is often pragmatic justification for graphic presentation of time *versus* the logarithm of residue concentration, the Working Party cannot recommend its use on a conceptual basis. This is not a denial of the fact that, in general, the rate of decrease of concentration of pesticide residues from crops can be reliably predicted, particularly at lengthy intervals subsequent to pesticide application.

## APPENDIX II: Terminal Residues of Cyclodiene Insecticides

Some recent developments in relation to the natures of terminal residues of the cyclodiene insecticides are summarized in the following sections.

*Biotransformation by Micro-organisms.* The action of micro-organisms upon the cyclodiene insecticides plays a very important role with regard to their persistence in the environment. It is now well established that biotransformations do occur under both aerobic and anaerobic conditions.

HILL and MCCARTY<sup>1</sup> found that aldrin, heptachlor, and endrin are rapidly broken down in sewage sludge under anaerobic conditions. Heptachlor epoxide and dieldrin show degradation, but much more slowly. They did not identify any of the products. In the case of heptachlor one product had a much shorter retention time on a DC-200 gas chromatographic column, and in the case of endrin at least four products were observed.

TU, MILES and HARRIS<sup>2,3</sup> studied the action of soil micro-organisms on aldrin and heptachlor. Ninety-two pure cultures were screened. The great majority showed conversion of aldrin to dieldrin and heptachlor to heptachlor epoxide. A number of fungi, actinomycetes, and bacteria which convert aldrin to dieldrin also convert dieldrin to other products, which were not identified. Some micro-organisms apparently converted aldrin directly to other products than dieldrin. In aqueous media heptachlor was hydrolysed chemically to 1-hydroxychlordene, and this compound was epoxidized by micro-organisms to 1-hydroxy-2,3-epoxychlordene and then converted to an unknown metabolite. Another pathway for heptachlor degradation was dechlorination to chlordene by bacteria and subsequent microbial epoxidation to chlordene epoxide.

WEDEMEYER<sup>4</sup> showed that the ubiquitous bacterium *Aerobacter aerogenes* converts dieldrin to the 6,7-trans dihydroxydihydroaldrin. Identification was based upon gas chromatographic and thin-layer chromatographic comparisons with authentic diol prepared by acid hydrolysis of dieldrin. He saw no further transformation of the diol.

MATSUMURA and his colleagues<sup>5,6</sup> isolated a number of microbes from soils that could degrade dieldrin. Water-soluble metabolites were formed, including some acidic compounds, and a number of additional metabolites were extractable by chloroform. Using a specially active micro-organism isolated from a soil sample from the Shell Chemical Co. manufacturing plant near Denver, Colorado, they observed at least nine metabolites. The five principal compounds were isolated from the soil sample and were characterized, as shown in Fig. 1, on the basis of infrared and mass spectra and chemical tests. Aldrin (metabolite J) was definitely formed from dieldrin and metabolite D seems well confirmed as an aldrin diol. This was the first

Fig. 1 Proposed Dieldrin Degradation Pathways  
by a Soil Micro-organism  
(Matsumura, Boush and Tai<sup>6</sup>)

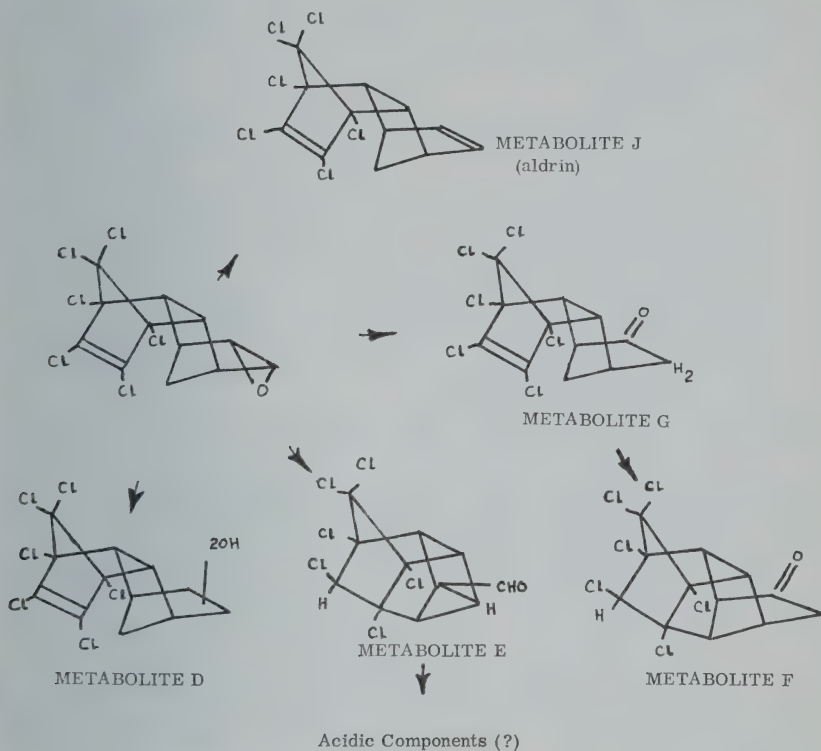
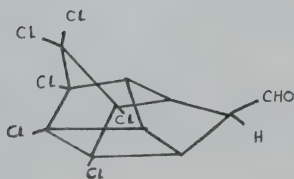


Fig. 2 Proposed Alternative for Matsumura Metabolite E  
(Rosen)





report of the dieldrin ketone isomer appearing as a metabolite of dieldrin, and it would be desirable to compare the metabolite G directly with the authentic compound (see SKERRETT and BAKER, *Analyst* **84**, 376 (1959); *Analyst* **85**, 184 (1960)). Metabolite F, since it can be formed from G by ultraviolet radiation seems well characterized if the identity of the latter is confirmed. The tentative structure assigned to metabolite E would be unexpected, and further characterization is desirable. ROSEN<sup>7</sup> has suggested the alternative structure shown in Fig. 2, which is in accord with the observed facts and with well documented pentacyclo (5 3 0 0<sup>2,6</sup> 0<sup>3,9</sup> 0<sup>5,8</sup>) decane ring systems.

KORTE and his associates<sup>8</sup> have applied the photo-isomer of dieldrin (Fig. 4, structure I) labelled with carbon-14 to culture media of *Aspergillus flavus* and *Penicillium notatum*. After 3 weeks 44.5% of the radioactivity applied to *Aspergillus flavus* was found in the mycelium and 37.5% in the culture medium. The percentage of the photo-isomer metabolized was 39% in the mycelium and 37% in the medium. In the case of the *Penicillium notatum* 79.6% was found in the mycelium and 9.5% in the medium. Percentages metabolized were 20% in mycelium and 48% in solution. There were two hydrophilic metabolites which have not yet been identified.

*Transformations On or In Plants.* A number of studies on plant metabolism of cyclodienes are in progress under the direction of KORTE<sup>8</sup>. The following paragraphs summarise recent progress.

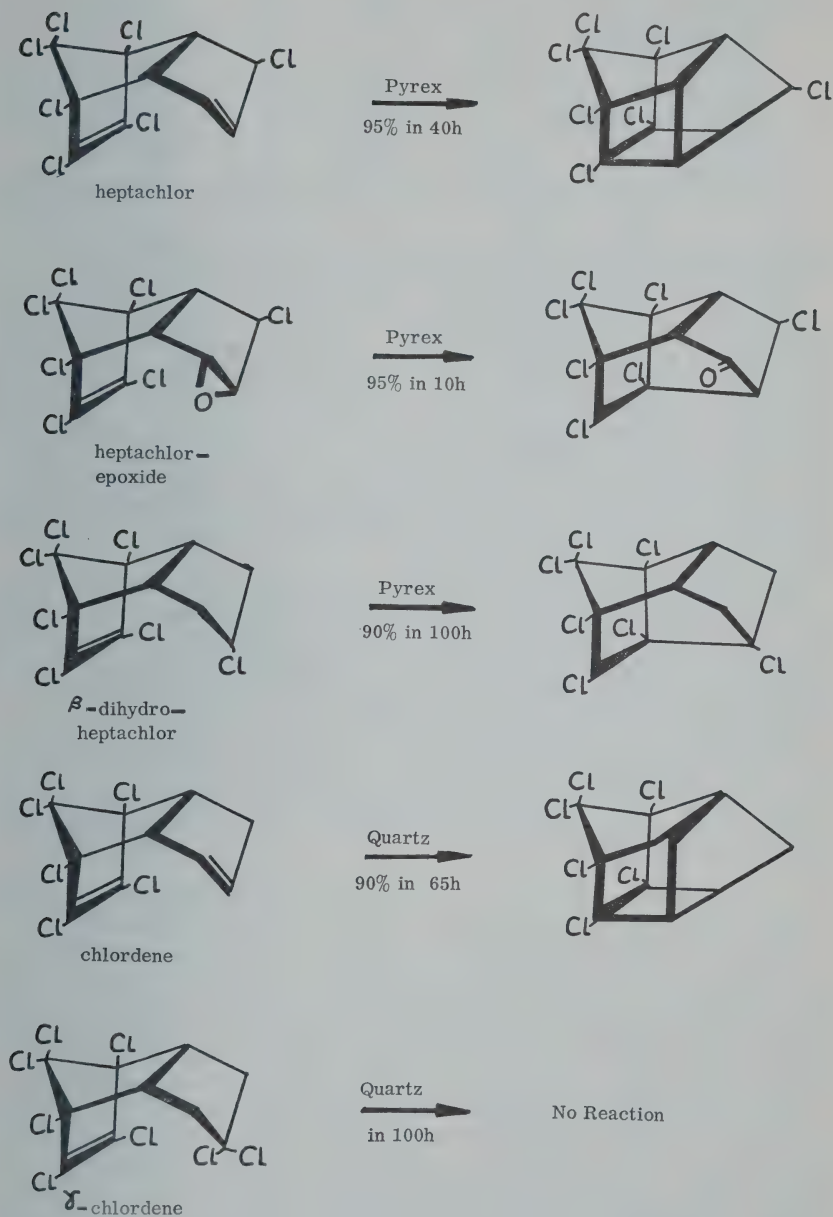
Investigations were carried out with aldrin-(<sup>14</sup>C), dieldrin-(<sup>14</sup>C), photodieldrin-(<sup>14</sup>C), endrin-(<sup>14</sup>C), isodrin-(<sup>14</sup>C), and lindane-(<sup>14</sup>C). Four weeks after application of *ca.* 75 ppm (based on weight at application time) of aldrin-(<sup>14</sup>C) on the upper side of the leaves of cabbage, only 17% of the applied radioactivity was recovered in plants and soil; 76% of the recovered activity consisted of hydrophilic metabolites. Besides aldrin, five other compounds were found. The less polar compound, which is Rf-identical with dieldrin, is found in only small percentages in the radioactivity in and on the plants, but the activity found in soil consists of 64% of it. Therefore, it is possible that this compound is formed by soil micro-organisms more quickly than by higher plants. The other compounds are very hydrophilic and are in all plant extracts in high amounts. The most hydrophilic ones are hydrolysed by methanolic HCl to less polar compounds, which have not yet been identified.

After application of dieldrin-(<sup>14</sup>C) in the same manner on cabbage, 40% of the radioactivity is recovered after 4 weeks; 34% of the recovered activity is due to at least two hydrophilic metabolites.

When photodieldrin-(<sup>14</sup>C) was applied on the leaves of cabbage, there was a steady decrease of the activity on the surface and a steady increase of the activity in the inside of the plant during 4 weeks. The activity found in the soil increased during the same time. While the activity on the surface of the plant was mostly due to unchanged photodieldrin, the activity extracted from the plant organs contained a metabolite which was more hydrophilic than both metabolites found by experiments with fungi. The total metabolism rate was up to 33%.

Endrin-(<sup>14</sup>C) was applied on the leaves of cotton (total *ca.* 120 ppm in three applications); 83 days after the last application the following percentages and concentrations of radioactivity were found in and on the organs and in the soil:

Fig. 3 Irradiation in Acetone with a HPK 125/Philips Lamp.  
(Korte et al. <sup>8</sup>)



Sample	Endrin, ppm	Recovered activity, %
dead leaves rinse	129.0	31.5
dead leaves extract	72.2	17.7
live leaves rinse	19.5	16.2
live leaves extract	17.1	14.3
stalks extract	0.33	0.27
roots extract	n.d.	n.d.
cotton fibre extract	0.36	0.0033
seeds extract	<0.1	<0.001
soil extract	0.0053	20.0

Besides endrin, a main metabolite was found which was only a little more hydrophilic than endrin itself, and three byproducts of high polarity.

The following preliminary results were obtained from experiments with *isodrin*-( $^{14}\text{C}$ ) on the leaves of cabbage. Thin-layer chromatography of the rinse showed a main metabolite with a chromatographic behaviour like endrin, and at least two very hydrophilic byproducts. Chromatography of the extract of the leaves showed a high percentage of very hydrophilic metabolites. Wheat-seedlings grown in water containing *lindane*-( $^{14}\text{C}$ ) metabolised the insecticide to a small amount to a very hydrophilic metabolite. After soil application to carrots and spinach and foliage application to spinach and cabbage, no metabolites were found in the soils, while all plant extracts contained a hydrophilic metabolite with a chromatographic behaviour similar to that of the wheat metabolite.

During the past year SAHA<sup>9</sup> has further studied the fate of dieldrin- $^{14}\text{C}$  in wheat plants grown in treated soil. Plants harvested 3 weeks after seeding contained a small amount of radioactivity, of which 98% was dieldrin, as evidenced by thin-layer chromatography in six different solvent systems and by gas-liquid chromatography. He concluded that root-absorbed dieldrin in wheat plants is less than 2% metabolised to other products.

WHEELER<sup>10</sup> has found that dieldrin is absorbed from an aqueous medium by *Chlorella*. The cellular portion contained increasing amounts with time, and more exhaustive extraction was required for its removal. Thin-layer chromatography indicated only dieldrin present after 72 hr. No apparent transformation had occurred.

**Photochemical Transformations.** KORTE<sup>8</sup> obtained the transformations shown in Fig. 3 upon irradiating acetone solutions of various cyclodienes.

ROSEN<sup>7</sup> has also found the same photo-isomer of heptachlor is produced by irradiation in the presence of benzophenone. Although he has not yet determined that the same conversion occurs in sunlight, he feels it is obvious that the same mechanism (triplet state) is operating in this case as in photo-aldrin and photodieldrin. He has found the photo-isomer of heptachlor to be more toxic to flies (2x) and to mosquito larvae (3x) than heptachlor.

Some additional data have been obtained by Shell Research Ltd., Tunstall Laboratories, on the occurrence of dieldrin photo-isomer (Fig. 4, No. 1) in a variety of samples. The results summarized in Table I, show measurable amounts only in samples of English lanolin. Human diets in Britain are apparently free from the compound, and none was detected in human fat samples. Further information regarding animal metabolism is presented in a later section.

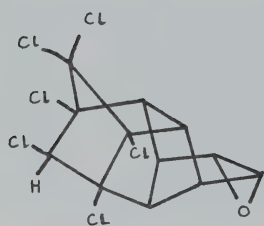


Table I—The Concentrations of HEOD and Dieldrin Photo-isomer in Selected Samples

Sample		Date	Concentration of residue, <i>ppm</i>		Sensitivity, <i>ppm</i>
			HEOD	dieldrin UVCP	
Human Fats					
British	1	April-May 1968	0.04	n.d.	<0.001
	2	"	0.07	n.d.	<0.001
	3	"	0.10	n.d.	<0.003
	4	"	0.06	n.d.	<0.011
	5	"	0.10	n.d.	<0.001
	6	"	0.26	n.d.	<0.003
	7	"	0.11	n.d.	<0.001
	8	"	0.13	n.d.	<0.002
	9	"	0.36	n.d.	<0.004
	10	"	0.08	n.d.	<0.006
	11	"	0.15	n.d.	<0.002
	12	"	0.14	n.d.	<0.003
	13	"	0.12	n.d.	<0.007
Human Fats					
Dutch		1967	0.13	n.d.	0.003
Heron Eggs		Spring 1967	0.73	n.d.	0.003
Chicken Eggs	1	May 1968	0.010	n.d.	<0.001
	2	"	0.006	n.d.	<0.001
	3	"	0.005	n.d.	<0.001
	4	"	0.004	n.d.	<0.001
	5	"	0.009	n.d.	<0.001
Mutton Fat					
English		May 1968	0.39	n.d.	0.004
New Zealand		"	0.009	n.d.	0.004
Lanolin	1	1966	41.0	5.8	—
	2	"	37.2	6.25	—
	3	"	11.6	4.66	—
	4	"	38.1	5.66	—
Human Diets		23.3.67	0.028	n.d.	0.002
		4.4.67	0.018	n.d.	0.002
		20.4.67	0.019	n.d.	0.003
		3.5.67	0.013	n.d.	0.001
		23.5.67	0.016	n.d.	0.002
		6.6.67	0.013	n.d.	0.001
		21.6.67	0.007	n.d.	0.001
		3.8.67	0.013	n.d.	0.006

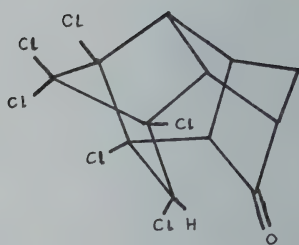
n.d. = none detected.

Fig. 4



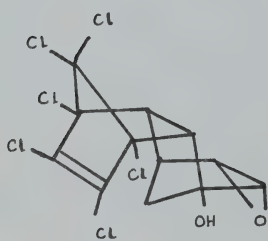
I

Dieldrin  
Photo-isomer



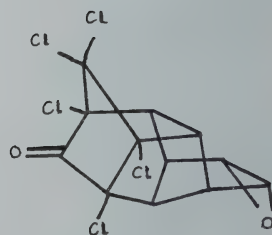
II

Endrin  
Keto-isomer



III

Dieldrin Rat Faeces Metabolite



IV

Dieldrin Rat Urine Metabolite

*Metabolism in Animals and Insects.* KORTE and his associates are continuing their work with the cyclodiene insecticides in insects and animals. The following paragraphs summarise their recent experience.

Investigations were carried out with photodieldrin-( $^{14}\text{C}$ ), endrin-( $^{14}\text{C}$ ) and aldrin-trans-diol-( $^{14}\text{C}$ ).

After intravenous injection of 70  $\mu\text{g}/\text{kg}$  of photodieldrin-( $^{14}\text{C}$ ) male rats had excreted 15.2% of the activity in faeces and 1.5% in urine after 72 hr, while female rats excreted 14.9% in faeces and 0.4% in urine. The activity consisted in larger amounts of hydrophilic metabolites; 60% of the activity which had remained in the body was found in the fatty tissues (abdominal fat, muscle, subcutaneous fat, and skin) and consisted mainly of unchanged photodieldrin. Faeces of both male and female rats contained two metabolites in the ratio 2:1 besides 5% of unchanged photodieldrin.

After intravenous injection of 115  $\mu\text{g}/\text{kg}$  of photodieldrin-( $^{14}\text{C}$ ) in male rabbits, 14.6% of the activity is excreted in urine and 1.7% in faeces within 4 days. The extracted radioactivity contains the same hydrophilic metabolites as in experiments with rats.

After intravenous injection of endrin-( $^{14}\text{C}$ ) in rabbits, four hydrophilic metabolites were excreted in urine. Feeding experiments with aldrin-trans-diol-( $^{14}\text{C}$ ) to rats showed that after 24 hr the activity in the faeces consisted of more than 90% of unchanged diol. A very hydrophilic main metabolite was observed besides at least two byproducts in very small amounts.

Metabolism of photodieldrin-( $^{14}\text{C}$ ) was studied with larvae of *Aedes aegypti*. Its dependence on time, application rate, and number of sub-lethal applications was measured. During 48 hr, the metabolism rate rises from 29% after 12 hr to 58% in the aqueous medium, while the metabolism rate in the larvae is reduced from 15% to 6.0%. Increasing application dosages (0.001-0.009 ppm) lead to a decreasing metabolism rate in the aqueous medium (53% to 32%). It increases again to 54% by using a lethal dosage; using a super-lethal dosage it increases to 46%. A lower concentration of larvae gives a lower metabolism rate in the aqueous medium. After five applications (altogether 0.003 ppm), metabolism rate in the solution was lower (31%) than after one application of 0.003 ppm (48%). Metabolism rate in the larvae was 6-7% in both cases. One main metabolite with a chromatographic behaviour very similar to photodieldrin was found, besides a very hydrophilic byproduct.

The Tunstall Laboratories of Shell Research Ltd. are also actively studying animal metabolism of endrin, dieldrin, and dieldrin photo-isomer.

In rats, RICHARDSON, ROBINSON and BALDWIN<sup>11</sup> of the Tunstall Laboratories, found that endrin is rapidly metabolized and excreted, as previously reported by KLEIN *et al.*<sup>12</sup>. They found three principal metabolites, one in the tissues and two in the faeces. None of these was the keto-isomer of endrin (Fig. 4, II), and they have not yet been identified. The  $R_f$  values of the keto-isomer and one of the fecal metabolites are very close on the thin-layer systems previously used by KLEIN, and retention times on the GLC column used by KLEIN for keto-isomer and one fecal metabolite are identical. These observations are thought to account for the apparent discrepancy between the work at Tunstall and that of KLEIN, and it is concluded that the delta-keto-isomer is not an important metabolite of endrin in rats.

Further work at Tunstall on the fecal metabolite of dieldrin in rats provides further support for its assignment as a monohydroxylated dieldrin, as shown in structure III, Fig. 4. The hydroxyl has been assigned to the five position on the basis of its strong effect on the  $\text{CH}_2$  resonances in the NMR.

Also at Tunstall, rats have been fed dieldrin photo-isomer over a period of time and toxicological results will be assessed in the near future. One prin-



cipal metabolite was found in tissues and in urine, and this metabolite proved to be identical to the urine dieldrin metabolite previously reported<sup>13,14</sup> (structure IV, Fig. 4.) The formation of this metabolite from photodieldrin provides additional support for structure IV.

HEDDE *et al.*<sup>15</sup> and FEIL *et al.*<sup>16</sup> have reported feeding studies with carbon-14 labelled dieldrin in sheep. They found at least seven metabolites in the urine. Two of these were characterized as the 6,7-trans aldrin-diol and its glucuronide conjugate.

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### APPENDIX III: Terminal Residues of Chlordane

*Work in Progress.* A number of projects are in progress, but are at present incomplete, with respect to terminal residues of chlordane. A listing of items in progress is:—

#### (a) *Preparation of Manuscripts:*

- (i) Terminal Residues of Chlordane (I): Relationship to Technical Chlordane<sup>1</sup>.
- (ii) Terminal Residues of Chlordane (II): Weathering of Residues from Foliar Treatments with Technical Chlordane<sup>2</sup>.
- (iii) Terminal Residues of Chlordane (III): Characterization of Components of Technical Chlordane<sup>3</sup>.

#### (b) *Chemical Research in Progress:*

Isolation, identification, and properties of unknown metabolite(s) of chlordane in animals<sup>3</sup>.

#### (c) *Toxicological Investigations:*

To supplement chemical knowledge on residues, a series of pharmacological investigations on alpha- and gamma-chlordane are also in progress<sup>4</sup>.

*New Literature.* BEVENUE and YEO<sup>5</sup> have reported on changes in composition of technical chlordane dispersed in water or when vapors are exposed to water. The evolution of chromatographic patterns is similar to observations reported to this Commission and the authors suggest that the chlordane peaks, which we have called *signature peaks*, be used to quantitate residues. The authors appear to have been unaware of published IUPAC Commission reports<sup>1,2</sup>.

SAHA and LEE<sup>6</sup> report mass and infrared spectroscopic data on isolates from a commercial chlordane formulation (25% granules). Their interpretations confirm the identity of major components, but their identification of some minor components and their assignment of structures differ from the conclusions of other workers<sup>3,8</sup>.

CHAU and COCHRANE<sup>7</sup> have described specific chemical methods for gas chromatographic identification of several organochlorine pesticides, including constituents of technical chlordane. Additional identifications, effects of strong basic reagents, and structures of chlordanes (and others) are discussed by COCHRANE<sup>8</sup>.

To provide a reference for ascertaining continuing constancy of composition of technical chlordane, a brochure<sup>9</sup> has been compiled, containing physical, chemical and biological test methods, a statement of approximate composition, and specifications.

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#### APPENDIX IV: Terminal Residues of Carbaryl and Carbamate Insecticides

Since the 1968 report, no new terminal residues of carbaryl have been reported. Following injection of carbaryl into bean plants, DOROUGH and WIGGINS<sup>1</sup> observed a gradual rise in water-soluble conjugates up to 56% within 10 days after dosing followed by a decrease to 2% after 90 days. An unextractable fraction was found to increase continually until it reached 78% of the dose in 90 days. The water-soluble conjugated materials were acid hydrolyzed and yielded aglycones as was previously reported. The unextractable fraction was not examined further. The organosoluble fraction was only carbaryl. When water-soluble metabolites were administered to rats acutely, almost all was eliminated within 96 hr. One study<sup>2</sup> (reviewed by abstract) reported that carbaryl was more easily translocated than sumithion in cocoa seedlings. Both insecticides moved rapidly to growing leaves and tip regions although uptake was slow. Uptake of radioactivity was evident up to 35 to 45 days after treatment.

*Other Carbamates.* CASIDA and his coworkers<sup>3</sup> synthesized potential oxidative metabolites and compared them to compounds produced from *in vitro* (model) biological systems. In all cases the toxicological potency of the conversion products *in vitro* was less than the parent pesticide.

The nature of the Furan<sup>R</sup> (NIA 10242, 2,3-dihydro-2,2-dimethyl-7-benzofuranyl-N-methylcarbamate) metabolites detected in bean plants following injection again suggested that hydrolysis, oxidation, and conjugation were the major pathways in metabolism<sup>4</sup>. The major metabolite found 28 days after administration was a conjugate of 3-hydroxy-Furadan. Small quantities of 3-hydroxy-Furadan, 3-keto-Furadan and the conjugate were observed as well as conjugates of the corresponding phenolic products. A significant quantity of unknown conjugates (9% of the administered dose) and unextractable material (10% of the administered dose) were also reported. Residues of Furadan and its phenol in Coastal Bermuda grass dissipated to nondetectable levels within 14 days following foliar spray application<sup>5</sup>. However, residues of Furadan were stable in grass and corn silage stored for 30 and 55 days, respectively. Corn silage residues, when fed to lactating cows, were not transferred to the milk. This study, in light of the report that the major residues are conjugates, may not be the complete picture in terms of terminal residue concentration. Procedures used in this study to extract Furadan would not be useful for extracting all the terminal conjugated residue products.

Several investigators reporting on the metabolic fate of Temik<sup>R</sup> (2-methyl-2-(methylthio)propionaldehyde O-(methylcarbamoyl)oxime) confirm those studies reported in 1967 and 1968<sup>6,7,8</sup>. Temik<sup>R</sup> is rapidly converted to its relatively stable sulfoxide analog which undergoes further degradation by oxidative and/or hydrolytic routes. Temik<sup>R</sup> fed to a lactating cow resulted in radioactive residues in the milk as was originally reported in 1968.

A unique photochemical rearrangement was recently reported<sup>9</sup> using p-tolyl-N-methylcarbamate as a model compound. Following UV irradiation the model compound (an antiesterase agent) was converted to p-cresol and N-methyl-2-hydroxy-5-methylbenzamide (non-antiesterase agents). Similar conversions of pesticidal carbamates might be affected under natural conditions.

A bioconversion product of Banlate<sup>R</sup> (du Pont 1991, methyl-1-(butylcarbamoyl)-2-benzimidazolecarbamate) in rat urine was recently reported to be methyl-5-hydroxy-2-benzimidazolecarbamate<sup>10</sup>. The parent compound apparently underwent both a hydrolytic and oxidative conversion.



A study on the metabolic fate of Mobam<sup>R</sup> in rats confirmed data previously reported that the compound is rapidly hydrolyzed and excreted in urine and feces as conjugates of the hydrolysis products<sup>11</sup>. Identification of the terminal residual products was not complete.

Several new N-methylcarbamates have been granted tolerances by the US Food and Drug Administration<sup>12,13</sup>. These include Bux (a 3:1 ratio of 1-methylbutylphenyl-N-methylcarbamate: 1-ethylpropyl-phenyl-N-methylcarbamate; 66% meta isomers and 31% ortho and para isomers) and methomyl (Lannate, S-methyl-N-((methylcarbamoyl)oxy)-thioacetimidate). A portion of the unpublished data on terminal residues submitted in support of the tolerance request is presented.

The metabolic fate of the predominant isomer of Bux was generally found to follow the course of degradation observed with aryl N-methyl carbamates: oxidation and/or hydrolysis followed by conjugation. The parent compound was rapidly hydrolyzed in soil with a half-life of approximately 1 week. One oxidative metabolite was identified as m-(1-methyl-1-hydroxybutyl)phenyl-N-methyl carbamate. Stability of a granular formulation as compared with the soluble preparation was somewhat longer with a half-life of 3 weeks. Little, if any, translocation of the insecticide and/or its metabolites in soil was observed. Experiments, designed to examine the potential corn root absorption of the pesticide, showed no terminal carbamate residues in the plant.

Traces of radioactivity found in the plant were believed to be natural products resulting from incorporation of <sup>14</sup>C-degradation products. A more complete metabolic picture of Bux in and on plants has yet to be delineated.

The pattern of metabolism of Bux in rats again resembles that reported for other carbamates. Within 48 hr. 66% of the administered dose of carbonyl-labelled Bux was hydrolyzed (expelled as <sup>14</sup>CO<sub>2</sub>), 14% was present in urine, 3% in feces and about 5% present in the rest of the animal tissue. *In vitro*, Bux was shown to form two major oxidized products, the N-hydroxymethyl derivative and the 1-methyl-1-hydroxybutyl derivative (N-methyl and side-chain oxidation). Urinary waste products were predominantly conjugates of the latter compound.

Several studies on the disappearance of methomyl from soil indicate that after 30 days from 50-75% of the parent compound had dissipated. In a laboratory study, after 42 days half of the applied dose was present as methomyl, approximately 15% was an unextractable unknown product(s), and the rest was lost, presumably by volatilization. The metabolic fate in corn plants following foliar application resulted in approximately 11% of the dose washed into the soil, 43% volatile components, and 46% plant radioactive residues. Examination of the extractable residue showed traces of methomyl (1.6% of the dose) and one nonpolar metabolite (2.9% of the dose). The remaining residue consisted of unextractable materials and natural components resulting from reincorporation of the radioactivity following degradation.

The metabolism of methomyl in tobacco grown in nutrient solution containing 10 ppm of radioactive methomyl was examined. From 20 to 25% of the pesticide was translocated into the plant. Of the material translocated into the plant 75% of the <sup>14</sup>C label was eliminated as volatile components identified as CO<sub>2</sub> and acetonitrile. The residue was identified as consisting of methomyl (82%) polar and nonpolar extractables (18%) and a trace of an oxime. Following foliar application, methomyl was poorly translocated within the plant.

Metabolism of methomyl in cabbage resulted in 21% of the administered dose eliminated as volatile components and 77% of the dose remained as a

$^{14}\text{C}$  residue. A major part of the residue was extractable (54% of dose) into polar and nonpolar components. The nonpolar component was unchanged methomyl. The polar compounds again were neutral lipids and other natural components containing reincorporated radioactivity. No evidence for the presence of methomyl sulfoxide or methomyl sulfone was observed. Unlike Temik, a closely related analog which is oxidized to a toxic, stable compound, it appears that upon oxidation methomyl degrades rapidly to yield small fragments, acetonitrile,  $\text{CO}_2$ , and methylamine. Thus, the only terminal residue that would be expected for this compound should be the parent compound.

Metabolic studies on the fate of methomyl in the rat following an oral dose showed 25% of the dose eliminated as urinary components. The components were not identified although the parent compound, its sulfoxide and sulfone analogs, oxime hydrolysis products and/or conjugates were not observed. Acetonitrile and  $\text{CO}_2$  were the major degradation products expelled by the rat. These studies again indicate that methomyl might be the only terminal residue in mammals following application. Degradation, once initiated presumably through oxidation, is rapid and complete.

*Acknowledgment.* The major portion of this report was contributed by Dr. R. L. BARON, US Food and Drug Administration, and his efforts are gratefully acknowledged.

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### APPENDIX V: Terminal Residues of Organophosphorus Compounds

*Malathion.* As early as 1956, MARCH and coworkers<sup>1</sup> proposed malathion monocarboxylic acid as a mammalian metabolite of the insecticide. This was later confirmed by KRUEGER and O'BRIEN<sup>2</sup>. All workers in the field of

malathion metabolism have clearly recognized the existence of two isomeric monocarboxylic acids, but it was not known which of the two (or a mixture of both) was produced by mammals. CHEN, TUCKER and DAUTERMAN<sup>3</sup> have just reported the synthesis of the isomers, structural assignment based on NMR evidence, and isolation of the metabolite from rat urine and from a rat liver carboxyesterase preparation. The isomer produced exclusively, both *in vivo* and *in vitro*, is the *alpha* monoacid, *i.e.*, the carbethoxy group is attached to the methylene group in the succinate moiety.

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### APPENDIX VI: Chemical Nature of the Terminal Residues of Fumigants

**Ethylene Oxide.** A mixture of 90% CO<sub>2</sub> and 10% ethylene oxide (EO) was used to fumigate 4.75 tons of wheat containing 15.1% moisture over a period of 18 hr in a 6-ton capacity silo. A commercially recommended dosage of 3 kg of the mixture or 0.3 kg of EO, when applied at 22 °C, caused residues of EO in different parts of the silo averaging 10.6 ppm at the end of the fumigation period and 7.2 ppm after 1 hr of thorough aeration. A second fumigation of the same grain under the same fumigation conditions resulted in an average of 14.2 and 10.5 ppm, respectively (PFEILSTICKER *et al.*<sup>7</sup>). No analyses of ethylene glycol (EG) and ethylene chlorohydrin (ECH) which are possible metabolic residues, were made nor analyses of EO after prolonged aeration. An analytical method for determining residues of EO, ECH, EG, and diethylene glycol in date fruit is provided by BEN-YEHOSHUA and KRINSKY<sup>1</sup>.

A group of six commercial firms interested in residues caused by the use of EO for fumigating spices, herbs, seeds, and natural flavoring, conducted cooperative experiments to determine ECH residues (analytical detectability around 20 ppm) resulting from unspecified but typical commercial fumigation practices. Residues ranging from <25-2,800 ppm were found in 37 spices, the highest being in black pepper. Ninety-day feeding studies on rats, dogs, and monkeys indicated a no-effect level of 45 mg ECH/kg/day (HALL *et al.*<sup>2</sup>).

Residues of ECH produced from EO fumigation of flour, disappear within a week when freely aired but remain unchanged over long periods under sealed conditions (HEUSER *et al.*<sup>3</sup>). Cakes baked from flour containing ECH retained approximately 10% of the original ECH. Virtually the whole chloride content of the flour was changed to ECH when flour was treated with very high dosages of EO. Leaf tobacco treated with 16.67 mg/l EO for 12 hr contained 230 ppm of ECH. In flour containing inorganic bromide as a result of previous methyl bromide treatment, the major part was converted to ethylene bromohydrin by subsequent treatment with EO (HEUSER *et al.*<sup>4</sup>).

**Methyl Bromide.** Commodities such as wheat flour, wheat, yellow maize (corn), sorghum, rice paddy, groundnut (peanut) kernels, groundnut expeller cake, sultanas, and cocoa beans were fumigated with methyl bromide (MB) under controlled temperatures, moisture contents, exposure periods, sealing, and aeration conditions to determine the unchanged fumigant residue, using an analytical method sensitive to about 0.1 ppm of MB. The initial MB



content for a given commodity was related to temperature, moisture content, and gas concentration employed, but not to exposure. The rate of disappearance of MB from flour, cottonseed cake, wheat, maize, and sorghum was practically as rapid under sealed conditions as when freely aired at 25°C. After rapid initial desorption, the ensuing amounts of MB, when plotted as the logarithm of 1/ppm, were found to be linearly related to the time of airing. It was concluded that the rapid disappearance of fumigant from these treated foodstuffs, together with the usual aeration and further processing that would normally occur, makes the ingestion of unchanged MB by humans remote, but situations could arise where food containing free MB might conceivably be fed to animals (SCUDAMORE and HEUSER<sup>9</sup>).

**Ethylene Dibromide.** Radioactive tracer studies with 1,2-<sup>14</sup>C ethylene dibromide (EDB) show that it is rapidly metabolized by rats when given an acute oral dose of 100 mg/kg. Although primary metabolites isolated are cysteine conjugates it is assumed that they are formed by initial conjugation with glutathione as described by NACHTOMI<sup>6</sup> who also found sodium bromide as a metabolite (JONES and EDWARDS<sup>5</sup>). It is not known whether the above reactions occur in the gaseous state with plant proteins or amino acids.

Two hundred pound lots of corn (white maize) in Ghana were treated with 5 ml of EDB poured on three corn cobs and then distributed vertically in the corn in polyethylene bags. This is about 120 ppm of EDB, if evenly distributed (HEUSER *et al.*<sup>4</sup>).

**Carbon Tetrachloride.** RECKNAGEL<sup>8</sup> theorizes that carbon tetrachloride (CCl<sub>4</sub>) induced hepato-toxicity in rats is related to peroxidative decomposition of cytoplasmic membrane structure of structural lipids caused by the formation of the free trichloromethyl radical CCl<sub>3</sub> and monoatomic chlorine. Free radical attack on the polyunsaturated fatty acids is the first step in their peroxidative breakdown resulting in the appearance of intense diene conjugation absorption. Such conjugations were detected in rat liver microsomal lipids as early as 90 min after carbon tetrachloride poisoning (RECKNAGEL). Free radicals such as CCl<sub>3</sub> may also react with amino and sulfhydryl groups such as occur in cysteine and amino acids. It is not known whether such reactions occur in the gaseous state with plant proteins or amino acids.

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## APPENDIX VII: Fate of Organochlorine Pesticides in Vegetable Oil Processing

This paper evaluates the likelihood of the occurrence of organochlorine pesticide residues in human food as a result of prevailing practices in producing vegetable oil products. Two routes of conveyance of residues are considered: the direct route by consumption of the processed vegetable oil products and the indirect route through consumption of products derived from animals fed byproducts of the oil manufacturing process.

The production of edible oil follows this course. Oil-producing seeds (or beans) are either *pressed* or *solvent-extracted* to isolate the crude oils. These oils, generally inedible at this point, are subjected to a multistage treatment to produce the finished edible oil or shortening. They are *alkali-refined*, *bleached*, *deodorized* and, if hardening is desired, *hydrogenated* in that order<sup>15</sup>. (Typical unit processes are described in Appendix VIIA.)

Three byproducts may become constituents of animal feed. These are: (1) oil seed meal from the *extraction* process; (2) soap stock from the *alkali-refining* step; and (3) condensate from the *deodorization* process.

Crude oils, even though themselves inedible, receive considerable attention with respect to their pesticide content. Frequently the finishing processes are performed at plants that are far from the extraction facilities, and crude oils may be transported across political boundaries. Inspections here may reveal residues of organochlorine compounds which, being lipophilic, concentrate in the crude oil. Tolerances and practical residue limits established for pesticides in crude oils should take into account the substantial changes in levels which result from typical processing.

While organochlorine levels may be increased in the oils (compared to the source crop), they are decreased in oil seed (or bean) meals by the *extraction* process. Since the meals are used in animal feeds, risk of transmitting these pesticides to the human food chain via animal products is diminished<sup>4</sup>.

Accumulating evidence now shows that residues of organochlorine pesticides are removed from the oils themselves in commercial refining. Such observations<sup>11</sup> contributed to the FDA's establishing tolerances for residues of DDT and toxaphene in soybeans, as well as in crude soybean oil moving in inter-state commerce, in the United States. GOODING<sup>10</sup> has shown through pilot-plant and commercial-scale production studies that up to 14 organochlorine pesticides were removed in the *deodorization* and *hydrogenation* stages of vegetable oil processing. (These 14 compounds are: aldrin, BHC, chlordane, DDT, dieldrin, heptachlor, heptachlor epoxide, kelthane, lindane, methoxychlor, sesone, strobane, TDE or DDD, and toxaphene.) SMITH *et al.*<sup>14</sup> confirmed these observations in a pilot plant study on cottonseed oil and soybean oil containing 7 organochlorine pesticides, one of which (endrin) was not included in the study by GOODING. BARRENTINE and CAIN<sup>2</sup> also demonstrated the simultaneous removal of endrin, toxaphene, and DDT from vegetable oil during *deodorization* in commercial-scale observations. Neither *alkali-refining* nor *bleaching* stages of processing have major effects on the organochlorine pesticide levels of the oils<sup>14</sup>.

Two properties of chlorinated hydrocarbons make them susceptible to the removal by commercial treatment: volatility<sup>13</sup> and susceptibility to dechlorination in the hydrogenation process. *Deodorization*, which is a vacuum-steam distillation, removes the organochlorine pesticides with the volatile fraction. During *hydrogenation* organochlorines are probably converted to chlorine-free organic compounds<sup>14</sup>. This hypothesis, while not demonstrated specifically for pesticides, has been shown to occur with similar organo-

chlorine compounds<sup>16</sup>. Adsorption by activated carbon in the hydrogenation catalyst has also been suggested as the mode of removal of pesticides<sup>10</sup>.

Pesticide monitoring in foods and feed confirm that finished vegetable oil products are very low in organochlorine pesticide content and that there is no disproportionate occurrence of organochlorine compounds in vegetable oil, fats, and shortenings. US food surveys<sup>3-9,12</sup> showed that this group contributes a maximum of 0.002 to 0.004 mg daily intake of combined organochlorine compounds representing 2.5% to 3.7% of total daily intake from all foods. The diet composite (1964-7) consisting of salad oil, mayonnaise, shortening, and peanut butter averaged a combined organochlorine pesticide level of about 0.02 ppm. The surveys showed that finished oil (and oil seed meals) contains significantly lower levels of chlorinated hydrocarbons than do the crude oils. None of the chlorinated hydrocarbons (except DDT and BHC occasionally) were found in oleomargarine, which is largely hydrogenated oil<sup>4</sup>. The exceptions are likely to have been introduced as a result of non-agricultural use of pesticides—after processing. (Total diet studies in England and Wales<sup>2</sup> do not shed light on the fate of organochlorine in vegetable oil processing, since animal and vegetable products are not separated in the category *Fats, etc.*, of the existing reports.)

By comparison with the level of organochlorine compounds in the *Oil, Fats, Shortening* food category, bromides occur more frequently and at average levels exceeding those of organochlorines roughly 100-fold, sometimes considerably more<sup>3,6,7,12</sup>.

With respect to possible effects on animal feed from use of oil-process byproducts relatively little is known except for seed and bean meals. From the controlled experiments<sup>10,14</sup> it seems unlikely that significant quantities of the chlorinated hydrocarbons may be introduced, but further study is required. The *alkali-refining* step is relatively inefficient in removing organochlorine compounds from the main body of oil. Therefore, the low concentration of these substances in the byproducts, which may be mixed into animal feeds, is not likely to be a relatively important source of contamination. On the other hand, the condensates from the *deodorization* process are potentially the site of greatest concentration of organochlorine pesticides. Pilot plant studies<sup>14</sup> indicate that this is not an efficient step and that considerable losses of the pesticides occur. However, the recovery of pesticides in these fractions in typical commercial production and the extent to which they may be incorporated into animal feeds is unclear at this time.

*Summary.* Some byproducts, for example soap stocks or fatty acids from *alkali-refining*, and condensates from *deodorization*, may be mixed into animal feeds, and their importance as routes of conveyance of organochlorine compounds is uncertain. Meals (cakes), byproducts of the seed or bean extraction processes, are also used in animal feeds but their organochlorine content is generally very low, and they are not considered an important source of these pesticides in the human food chain. Typical commercial processing of edible vegetable oil products removes organochlorine pesticides from the portion consumed directly by humans.

#### *Appendix VIIA: Unit Processes in Edible Oil Manufacture*

*Alkali-refining.* A vigorously agitated treatment of the oil with aqueous alkali in excess of the equivalent free fatty acid content, at 135-150°F (57-66°C), for 30-40 min, followed by washing with water at 170-180°F (77-82°C), and drying through sparging with nitrogen for about 1.5 hr at 210-220°F (99-104°C).



**Bleaching.** Stirring with 0.5 to 1.5% of activated clay, carbon, and diatomaceous earth at about 180°F (82°C), followed by filtration through a bed of similar material as a filter medium.

**Hydrogenation.** Reaction with hydrogen in the presence of nickel catalysts on clay and carbon supports (approximately 0.05% of weight of oil) under hydrogen pressure of approximately 35 lb/sq. inch (180 cm of Hg) at about 350°F (177°C).

It should be noted that the hydrogenation is applied in the processing only of oils which require *hardening*.

**Deodorization.** Batch or semi-continuous treatment of oil by passage of water vapor through the oil for approximately 2 hr at 440-490°F (227- 254°C) under vacuum (5-7 mm of Hg). The amount of water passed through the heated, evacuated mixture corresponds to a rate per hour of 4-5% of the weight of oil being processed. This vacuum-steam distillation removes 5-10% of volatile constituents of the oil.

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### APPENDIX VIII: Effects of Washing, Cooking, and Other Processing on Residues of Organochlorine Pesticides

Although most tolerances for pesticide residues are established on the raw agricultural products, the objective always is to minimize and keep at a safe level the quantities of pesticides consumed with one's food. A number of studies have been made to show the changes in residue content as foods are processed from their harvesting through washing, cooking, and/or manufac-

turing procedures in preparation for our dinner table. STOBWASSER *et al.*<sup>1</sup> have recently published an excellent review article on this subject listing 95 references. A large number of pesticides including fungicides and organophosphorus insecticides are included.

The review below covers only organochlorine pesticides but does describe studies on dairy products, poultry, vegetable oils, *etc.*, as well as fruit and vegetables.

*Fruits and Vegetables.* There have been more studies made on the fate of DDT residues during processing than on any other pesticide.

The National Canners Association (NCA) has been conducting a series of well-planned experiments on residues of DDT and several other widely used pesticides. FARROW and coworkers<sup>2</sup> studied losses of DDT (as well as malathion and carbaryl) from tomatoes during processing. Starting with field-sprayed tomatoes containing approximately 7 ppm total DDT (p,p'-DDT, +o,p'-DDT, +p,p'-DDE) and following normal commercial preparative procedures, they found that the water wash removed from 85 to 92% of the residue. It made little difference whether detergent was or was not used. With the subsequent removal of the peel, either by steam peeling for whole peeled tomatoes or by screening in production of tomato juice, removal of DDT residue was 99% or better with only a trace remaining. Starting with technical DDT containing approximately 27% o,p'-DDT and 64% p,p'-DDT, they found a higher ratio of o,p'-DDT to p,p'-DDT after washing. In skins and waste from juicing operations almost equal amounts of o,p'-DDT and p,p'-DDT were found. These workers also studied removal of residues by home preparative steps and found the washing less effective than in commercial processing. From an original total residue of 4.4 ppm, 0.94 ppm remained after cold water wash, a reduction of 78%. Peeling after immersion in boiling water removed practically all of the remaining residue. In the home preparation of stewed tomatoes only about 85% of the residue was removed.

LAMB and coworkers<sup>3</sup> at NCA reported on the behavior of DDT in potatoes during processing. Potatoes were grown in soil which had been treated with DDT over a 5-year period. Based on organic chlorine content analysis the soil contained about 10 ppm of DDT. The potatoes at harvest contained about 0.5 ppm total DDT (p,p'-DDT + o,p'-DDT + p,p'-DDE). Commercial washing removed about 23% of the residue and lye peeling plus washing about 94%. After canning and processing only a trace of residue remained. In home preparation, peeling removed over 90% of the residue but boiling or pressure cooking of the potatoes with skins resulted in no significant reduction of residues.

In 1966 FARROW and coworkers<sup>4</sup> at NCA reported that p,p'-DDT was partially converted to p,p'-TDE during the processing of canned spinach. Starting with 10 ppm of DDT at 250°F the p,p'-TDE level reached a maximum in 6 min when it was about equal to the p,p'-DDT concentration. With increased time of processing the combined DDT and TDE concentration gradually decreased. The conversion took place in spinach processed in plain tin plate, enamelled tin plate, and glass containers.

In 1968 LAMB and coworkers at NCA<sup>5</sup> reported on the removal of DDT (as well as parathion and carbaryl) from spinach by commercial and home preparative methods. Spinach was sprayed with DDT 50% wettable powder at the rate of 6 lb/acre and harvested 13 days later. This was a shorter pre-harvest interval than the registered use calls for and residues at harvest were about 25 ppm total (p,p'-DDT + o,p'-DDT + p,p'-DDE). In the commercial processing minimum washing reduced the residue by 17%, maximum washing by 48%, and maximum washing with detergent by 73%. Steam or water

blanching did not significantly decrease the residue of the washed spinach. Again, it was noted that the p,p' isomer of DDT decreased more than the o,p' during washing and blanching. Analysis of the canned spinach about 5 months later showed no DDT and only small amounts of p,p'-TDE and p,p'-DDE. The overall reduction in residue was over 90%.

In home preparation, washing removed about 30% of the total DDT, blanching about 52%, but cooking the spinach using only the water adhering after the wash decreased the residue only 39%. With the limited amount of heating involved p,p'-DDT did not convert to p,p'-TDE.

ELKINS and coworkers at NCA<sup>6</sup> studied the removal of DDT (as well as malathion) from green beans. Field-sprayed beans were used which contained about 4 ppm total DDT at harvest. Washing and blanching removed about 50% of the residue. In every case, more of the p,p-isomer was removed than of the o,p'-isomer. After canning and processing over 80% of the total DDT residue had been removed. Again, some p,p'-DDT was converted to p,p'-TDE. The beans used for the home preparative studies contained about 13 ppm total DDT. A cold water wash carried out 1 day after harvest removed 71% of the total DDT residue but 5 days after harvest only 52% was removed by the wash and 14 min boiling. After cold water wash and home canning over 80% of the total DDT residue had been removed.

CARLIN *et al.*<sup>7</sup> investigated the effect of commercial processing on residues of DDT in snap beans. The unwashed beans contained 3.6 ppm of DDT. After washing, blanching, and freezing only 1.4 ppm remained, a reduction of about 60%. After the canning process, no residue was found in the canned beans.

HEMPHILL *et al.*<sup>8</sup> studied the effect of home preparation on DDT residues in 3 market samples of green beans. The samples as obtained contained an average of 0.67 ppm total DDT. The washing and trimming each removed approximately 5% of the residue. They also noted that the loss of p,p'-DDT was greater than the loss of o,p'-DDT. After cooking, the total losses were 46% with 12 min boiling, 63% with 3 min pressure cooking, and 48% after 6 min electronic cooking. The boiling and pressure cooking partially converted p,p'-DDT to p,p'-TDE.

Using the Schechter-Haller colorimetric procedure, MENZER and coworkers<sup>9</sup> studied the effect of commercial canning process on residues of DDT in green peppers. The field-treated peppers contained from 3.2 to 8.4 ppm of DDT before washing. The first washing removed about 40% of the residue. After the second washing approximately 60% had been removed and the same level was found in the peppers in the can.

BRITTIN and FAIRING<sup>10</sup> studied the effects of processing on residues of methoxychlor and TDE. The products were fortified with added pesticide, cooked, pureed, and packed in glass containers under vacuum. They found that for methoxychlor added to peaches and peas at levels of 2 to 10 ppm approximately 95% of the pesticide was lost in the processing. Approximately 50% of TDE added to green beans at levels of 0.1 to 5.0 ppm was lost in the processing.

BLINN and coworkers<sup>11</sup> harvested lemons 33 days after the application of Tedion and found an average of 1.39 ppm of Tedion in the peel. A commercial washing operation, consisting of soaking the lemons for 2 min in a solution containing soap, borax, and boric acid, scrubbing with mechanical brushes in the same solution and then rinsing in clear water resulted in about a 60% reduction of the residue.

KLAYDER<sup>12</sup> added captan to asparagus, string beans, and spinach at levels of 10 to 120 ppm. After canning, the vegetables were heat processed at 14 psi,



the spinach for 1 hr and the asparagus and string beans for 35 min. In each case, over 95% of the captan was lost.

*Dairy Products.* With the acceptance and widespread usage of the electron capture-GLC detection for halogenated pesticide residues beginning in 1963, lower and lower levels of contamination were being detected and measured. Samples of milk and other dairy products which in earlier years might have been reported as free from pesticide residues were now being found to contain significant amounts of organochlorine pesticides and their alteration products. In addition to taking all practical steps to prevent contamination of the milk it also became important to know what happened to such residues as milk was processed into the various dairy products. Foremost among scientists studying these problems have been LISKa and his coworkers at Purdue University. In an excellent review article, LISKa<sup>13</sup> discusses the problem and work being done on it. He points out that the investigations are important from two aspects: (1) effects of normal processing on residues with (2) possible use of processing as a means of intentionally removing residues from foods.

LANGLOIS, LISKa and HILL<sup>14</sup> studied the effects of processing on residues of DDT and lindane and also of endrin, dieldrin, heptachlor, and heptachlor epoxide<sup>15</sup>. Feeding the respective pesticides (except heptachlor epoxide) to cows, they used the resulting contaminated milk to manufacture butter, ice cream, Swiss-type cheese, condensed milk, and dry whole milk, both by spray drying and by roller drying. In addition, they also used milk to which the pesticide was added directly. In general, they found that the pesticide residue concentration in the fat remained fairly constant during processing and that the residue went along with the fat. For example, milk containing 26 ppm of DDT (on a fat basis) resulted in a butter which after 4 months storage at -15°F showed 25 ppm of DDT, milk containing 20 ppm of DDT resulted in cheese containing 22 ppm of DDT. Lindane, perhaps because it is more soluble in the whey, did show a decrease of approximately 37% when milk containing 24 ppm was manufactured into cheese. A major reduction did take place when drastic heat treatment such as in the manufacture of roller- or spray-dried whole milk powder was involved. In these cases reductions of greater than 50% (fat basis) took place ranging from 52% for dieldrin to as high as 82% for lindane and DDT.

STEMP and LISKa<sup>16</sup> investigated the fate of telodrin and methoxychlor. They reported that 40-50% of telodrin residues were destroyed in preparation of evaporated milk and 10-20% in preparing dry whole milk. Methoxychlor was much more stable and showed a reduction of 25% in evaporated milk but practically no reduction in dry whole milk preparation.

MCCASKEY and LISKa<sup>17</sup> studied the behavior of endosulfan and chlordane during processing of milk. They found that when they fed endosulfan to a cow only endosulfan sulfate showed up in the milk. To cover both the metabolite and the parent pesticide they used both milk contaminated directly with the pesticide and milk contaminated by feeding the pesticide to the cow. Using milk containing about 15 ppm (fat basis) of the pesticide or metabolite, they found a reduction of 50% and 70%, respectively, of endosulfan and endosulfan sulfate in the manufacture of drum-dried whole milk while about 45% of the chlordane was lost.

MONTOURNE and MULDOON<sup>18</sup> at the University of Idaho manufactured 17 lots of cheese, cheddar and monterey, using milk from cows which were fed DDT-field treated hay. Samples were obtained from each phase of manufacture and analyzed using electron capture-gas chromatography. On a fat

basis the residue (total DDT and DDE and TDE) was about the same in the finished cheese as in the milk. One oddity noted was the great difference in composition of the residue in the whey as compared to the milk and cheese. No DDT was detected in the whey but the TDE content was much greater than in the milk or cheese.

	DDE	TDE	DDT (ppm fat basis)
milk and cheese	7.5	9.7	4
whey	10	29	0

There was no significant change in residue levels of cheese stored as long as 48 weeks.

LI, BRADLEY, and SCHULTZ<sup>19</sup> at the University of Wisconsin investigated the fate of residues of dieldrin, heptachlor epoxide (from feeding of heptachlor), DDT, lindane, toxaphene, chlordane, endosulfan, and kelthane during the manufacture of pasteurized whole milk, 30 % cream, butter, spray-dried whole milk, condensed whole milk, and cheddar cheese and their byproducts, skim milk, butter milk, and whey. The residues were introduced into the milk by feeding the pesticides to the cows. Their analyses again indicated that on a fat basis the residue concentration remained fairly constant except that there was a loss of residue in the preparation of spray-dried whole milk and that there was an increase in residue in skim milk, buttermilk, and whey. The increase in concentration of residues in the fat of low fat products has been noted by other workers<sup>14,15,18</sup>. LI and coworkers suggest that this might be attributable to the affinity of the residues for the phospholipid portion of the products.

Several workers have investigated the use of specialized techniques as a means of deliberately reducing residues in dairy products. KROGER<sup>20</sup> starting with milk containing naturally incurred (through the feed of the cows) residues showed that heating butter oil for as long as 1 hr at 120-130°C and 0.15 mm of Hg resulted in no measurable losses of heptachlor epoxide and dieldrin. However, using a steam deodorization process even 2 hr at 130-150°C at 2 mm of Hg resulted in 34 % reduction of heptachlor epoxide and 20 % reduction of dieldrin. Subjecting the butter oil to steam deodorization at 180-185°C and 0.01-0.5 mm of Hg for 5 hr resulted in complete removal of the pesticide residues. LEDFORD and coworkers<sup>21</sup> added pesticides to milk at the 0.5-ppm level (product basis) and found that passing the milk through a commercial process for removing off-flavors which involved steam heating and vacuum treatment removed 8 % of p,p'-DDT, 24 % of lindane, and 3 % dieldrin but did not remove any heptachlor.

LI and BRADLEY<sup>22</sup> investigated the use of high intensity UV light to destroy residues of pesticides in milk and butter oil. The products were exposed to UV light from a carbon arc as they were pumped over a surface cooler. Losses were much greater in the butter oil than in the milk; for example, 96 % of methoxychlor destroyed in butter oil vs. 33 % in milk. Methoxychlor was the most susceptible to change of the pesticides tests with others in decreasing order being DDT, kelthane, TDE, heptachlor epoxide, and dieldrin.

*Miscellaneous Products.* The removal of all residues of chlorinated pesticides during the processing of vegetable oils has been observed by several workers.

GOODING<sup>23</sup> reported that when a crude vegetable oil containing 2.8 ppm of chlordane, 0.5 ppm of DDT, and 0.5 ppm of TDE was subjected to a hydrogenation step during processing all the pesticides disappeared, presumably through adsorption by the activated charcoal contained in the catalyst or possibly by destruction by dehalogenation in the hydrogenation process. He also described another experiment in which the following concentrations of pesticides were added to a crude cottonseed oil, 1 ppm of aldrin, 15 ppm of BHC, 1 ppm of chlordane, 21 ppm of DDT, 1 ppm of dieldrin, 1 ppm of heptachlor, 1 ppm of heptachlor epoxide, 1 ppm of kelthane, 30 ppm of lindane, 42 ppm of methoxychlor, 18 ppm of sesone, 15 ppm of strobane, 21 ppm of TDE, and 21 ppm of toxaphene. The oil was tested at each stage of alkali-refining, bleaching, and deodorization. All residues had disappeared upon deodorization. The analyses were done using electron capture and microcoulometric methods.

SMITH *et al.*<sup>24</sup> described a study conducted under the auspices of the National Cottonseed Products Association in which crude soybean and cotton seed oils were processed using simulated commercial processing procedures. Two cottonseed oil samples were fortified with endrin, DDE, aldrin, dieldrin, heptachlor, and heptachlor epoxide at 1.0 ppm and DDT at 21 ppm. These samples, together with five soybean and five cottonseed crude oils were processed with analyses following each processing step. The analyses were made using electron capture and microcoulometric GLC with a method sensitivity of 0.03 ppm. Results indicated that alkali-refining or subsequent bleaching did not reduce the residue levels. Deodorization with or without hydrogenation eliminated all evidence of the chlorinated pesticides. Two soybean samples containing endrin were hydrogenated before deodorization and the endrin level was reduced near to or below the detection level of the method.

Several studies have also been made of the effect of cooking on chlorinated pesticide residues in chicken tissues. RITCHEY *et al.*<sup>25</sup> fed DDT and lindane separately and in combinations to chickens for 9 weeks. After slaughter, the birds showed residues of lindane, DDT, DDE, and kelthane in their tissues but not TDE. Baking at 350°F for 1 hr or frying for 45 min in an open pan resulted in reductions of the total residue by about  $\frac{1}{4}$  by baking and about  $\frac{1}{3}$  by frying. TDE was found in all of the cooked birds which had been fed DDT but not in the raw birds. Incidentally, it was noted that the presence of lindane resulted in more DDT being stored in the tissues.

LISKA and coworkers<sup>26</sup> fed several pesticides (DDT, lindane, dieldrin, endrin, and heptachlor) individually to hens and followed the fate of the resulting tissue residues through the cooking process. Although heptachlor was administered to the hens the residues were mainly heptachlor epoxide. Cooking in water at 190-200°F for 3 hr reduced the residues by up to 90%. The concentrations in the resulting fat drippings approximated those in the abdominal fat; however, the rate of rendering of fat and residues differed between light and dark meat. Heptachlor was held more tightly than the other pesticides and was only partially removed from the body tissues. Autoclaving the carcass at 15 psi for 3 hr removed essentially all residues except heptachlor, traces of which still remained (sensitivity of analysis 0.1 ppm using ECGC). The white meat after 3 hr of processing contained a higher level of heptachlor than the raw white meat but the lipid content also showed an apparent increase suggesting that the heptachlor increase may have been due either to a reabsorption from the environment or selective absorption from the fat drippings.



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## COMMISSION VI.5.2: PESTICIDE RESIDUE ANALYSIS

1. The Commission met on 3rd, 4th and 5th July. Those present were: GALLEY, ABBOTT, COOK, FREHSE, HURTIG, RESNICK, WIDMARK (Titular Members); BURNS BROWN, ELGAR, KOIVISTOINEN (Associate Members). An apology for non-attendance was received from MCCULLY (Associate Member).

2. The Chairman welcomed members and visitors to the meeting and moved the adoption of the agenda; this was agreed.

3. The Chairman referred to the minutes of the Third Meeting, held on 7-8th October, 1968, which, together with Appendices, had been circulated previously; with minor corrections which were indicated, these were agreed.

4. Arising from the minutes of the Third Meeting the following matters were referred to:

(a) It was reported that the proceedings of the Third Meeting had been published in the *Information Bulletin* No. 34, pp. 43-47, and that a summary report had been published in *J. Assoc. Offic. Anal. Chem.* **52**, 306 (1969). These reports had been distributed to Members and to interested agencies.

(b) Progress in liaison between IUPAC and the Codex Alimentarius and its Committee on Pesticide Residues, to which Dr. HURTIG had been asked to act as IUPAC spokesman, was reported. The work of a drafting working party of the Codex Committee on Pesticide Residues which met in Ottawa in June 1969 to discuss *referee methods of analysis* was noted. IUPAC might be asked by the Codex to elaborate such methods. The possibility of inter-laboratory collaborative studies in this connection was discussed.

(c) The FAO Status Report-1969, referred to in the minutes of the Terminal Residues Commission, was discussed in terms of analytical problems of interest to FAO, WHO, and Codex Alimentarius. Members distinguished between regulatory and referee methods and recognized that the former should be recommended by the Joint Meeting of Experts (FAO/WHO). The suggestion that a *Methods Manual* should be prepared was discussed in some detail. There was general agreement that the format of the FAO/WHO monographs should be standardized in respect of analytical methods with reference to an Appendix on multidetection methods as appropriate. It was also thought that greater guidance should be provided by FAO on the methods of analysis to be used at the tolerance levels recommended by the Joint Meeting.

(d) No report had yet been received on the progress of the OECD study. It was understood that Prof. WIDMARK would attend, as IUPAC observer, the meeting to be held in the Netherlands in September 1969 to discuss results of the latest analytical studies.

### 5. Organochlorine Compounds

(a) The Commission reviewed progress on the development of multidetection methods of analysis for residues of organochlorine pesticides. Based on the views expressed by members of a Working Party (Appendix I), the following recommendations were made:

- (i) That as an interim measure the Commission on Pesticide Residue Analysis should adopt the Mills' procedures as defined and explained in the *FDA Pesticide Analytical Manual*, Vol. 1, 1968, as multidetection methods which are suitable for recommendation to FAO, Codex Alimentarius, and other interested parties. It is also recommended that further consideration be given to the recommendation of at least one alternative multidetection method.

- (ii) That the Section attempts to promote the further development and orderly improvement of the Mills and other adopted methods.
- (iii) That research on the development of confirmatory tests which are compatible with adopted methods should be encouraged.
- (iv) That the Section publicizes and emphasizes the importance of expertise and experience on the part of the residue analyst applying any of these multidection techniques, particularly in view of the possible presence of interfering substances such as the polychlorobiphenyl (PCB) compounds.

With the recognition that other types of method may be more suitable for certain purposes, these recommendations were *agreed* by the Commission. The report and its recommendations were welcomed on behalf of FAO. Arrangements were made to continue to survey progress of work in this field. The collaborative work being undertaken at present by CE was also mentioned and the need for closer liaison was stressed. A report on the progress of a working party on pesticide residues within the COMECON organization was also discussed.

(b) The recent collaborative study on the determination of organochlorine pesticides in edible oils and fats, organized by the Oils and Fats Section of IUPAC, was discussed. It was agreed that the recommendations referred to above should be drawn to the attention of the Oils and Fats Section.

(c) Arising out of the FAO Status Report, the requirements for methods for endosulfan and toxaphene were discussed. Consideration of methods for toxaphene was deferred until the uniformity of the technical product can be more firmly established.

(d) The paper on chemical identity and confirmation of results by Dr. McCULLY (*World Rev. Pest Control* 8, 59 (1969)) was noted.

## 6. Organophosphorus Compounds

(a) The report of a Working Party on multidection methods of analysis for organophosphorus compounds was presented (Appendix II). Arising from this report, three recommendations were made:

- (i) That we defer at present the recommendation of multiresidue methods for organophosphorus pesticides and their metabolites.
- (ii) That we encourage laboratories to develop more validation data for the procedure utilized by ABBOTT *et al.* for total diet samples, the acetonitrile-charcoal method of STORHERR and WATTS, and other similar methods.
- (iii) That further confirmatory test techniques be developed—such as application of gel chromatography, two-dimensional thin-layer chromatography with oxidation or other chemical treatment between the two developments, the oxidation techniques of THORNTON and ANDERSON, and the use of multiple detector systems.

These recommendations were *accepted* by the Commission. Arrangements were made to continue to survey progress on multidection procedures for organophosphorus compounds.

(b) A review of other methods for a number of organophosphorus pesticide residues was also presented. No attention had been given to multidection methods nor to the separation and/or determination of mixtures of pure compounds without prior clean-up of plant or animal material. There was still a need for methods for individual pesticides and their metabolites, especially for such purposes as field trials, deciding tolerance levels, *etc.* A proposal to devise some questionnaires relating to such analytical methods as



a first step to an orderly presentation of the required data was gladly accepted by the Commission. Arrangements were made to collate information on the analysis of organophosphorus pesticide residues and to present the latest review in a form suitable for publication in *Pflanzenschutz-Nachrichten Bayer*. It was concluded that it was desirable that the analyst be provided, whenever possible, with information as to which metabolites and transformation and break-down products should be included in the residue methods. The vast field of organophosphorus compounds can only be handled adequately on the analytical side after definite border lines have been drawn. For the future, a working sequence of the order:

FAO/IUPAC Terminal Residues Commission  $\Rightarrow$  FAO/WHO Joint Meeting IUPAC Commission on Residue Analysis, should be aimed at.

(c) Some discussion occurred as to the place of conjugates, such as those of azodrin, bidrin, and carbaryl, in residue studies. It was felt that this important problem should be brought to the attention of the FAO/WHO Joint Meeting.

(d) FAO/WHO requirements for methods for organophosphorus compounds were considered in the light of recent reports. Work on phosphamidon, dichlorvos, malathion, and others was known to be in progress.

(e) Reference was also made to a screening method for organophosphorus pesticides, involving hydrolysis to dialkyl phosphate or phosphorothionate, methylation, and GLC examination of the resulting tri-alkyl ester (*J. Chromatog.* **41**, 180 (1969)).

## 7. Fumigants

A report on recent progress in the development of multidetection methods for fumigants (Appendix III) referred in particular to a scheme in which GLC, employing three types of detector, is used to analyse the contents of processed solvent extracts. Difficulties in determining residues of phosphine were discussed in particular. The extent and nature of the chemisorption of this compound is in doubt at present and it was agreed that this problem should be referred back to the Terminal Residues Commission. It was agreed that attempts should be made to arrange for an assessment of the multiresidue methods to be carried out in other interested laboratories such as those in Israel, Holland, Hungary, and Germany.

## 8. Rethrins and Synergists

A report had been received describing GLC and TLC procedures used for the analysis of residues of synergized pyrethrins in fatty meat. The method involves extraction, partition clean-up, elution through a Florisil column, chromatographic clean-up on Gelman glass microfibre strips, and GLC determination with electron capture detection (W. K. BRUCE, *J. Agric. Food Chem.* **15**, 178 (1967)). According to the FAO Status Report, the requirements of FAO/WHO for pyrethrin and piperonyl butoxide are now met. The suggested method was currently being validated in the USA; known difficulties in the GLC examination of extracts containing residues of pyrethrins were discussed.

## 9. Other Compounds

(a) *Dithiocarbamates*. The work on these compounds referred to in the minutes of the Terminal Residues Commission, was relevant. Studies on the development of analytical methods were in progress. Arrangements were made for a survey of methods for dithiocarbamates.

(b) The lists of compounds on the agendas of future FAO/WHO Joint Meetings were discussed with special reference to fungicides (1969) and herbicides (1970).

(c) A GLC method for chloropropylate and chlorobenzilate had been examined in one laboratory and found to be satisfactory.

### 10. Organomercury Compounds

(a) The Commission received a report on recent progress in the analysis of organomercury compounds (Appendix IV). The neutron-activation analytical method was now well validated for total mercury determinations and the use of atomic absorption methods was also making progress. It was recognized that these compounds were fairly widely used on a large scale in some developing countries.

(b) The development of an analytical procedure for the identification and determination of residues of organomercurial fungicides by thin-layer and gas chromatography was also reported. After extraction from the sample substrate (potatoes, apples, and tomatoes) with slightly alkaline cysteine hydrochloride in propan-2-ol, the mercurials are converted to their dithizonates for chromatographic examination. Details of this work are published in *J. Chromatog.* **44**, 284 (1969) (J. O'G. TATTON and P. J. WAGSTAFFE).

(c) The intended production by IAEA of a booklet on various aspects of mercury in the environment, including analytical material, was noted. General discussion also ranged over similar problems observed with lead, copper, tin, selenium, and sulphur compounds.

### 11. Publication

The secretary was authorized to arrange for publication of the proceedings of the Commission by IUPAC and for a summary to be published in *J. Assoc. Offic. Anal. Chem.*

### 12. Arrangements for Next Meeting

It was announced that the next meeting of the Commission would be held at Ingelheim, Germany, from 14th to 18th September, 1970.

### *APPENDIX I: Multiresidue Methods of Analysis for Organochlorine Compounds*

At the Third (1968) Meeting of the IUPAC Commission on Pesticide Residue Analysis, it was agreed that a Working Party be convened to investigate the advantages and disadvantages of the current multiresidue systems for organochlorine and organophosphorus pesticide residue analysis, with a view to determining the methods that were most fully investigated and best supported so that a recommendation could be made from IUPAC for use by interested parties in routine residue analysis. A Working Party composed of Prof. G. WIDMARK, Dr. D. C. ABBOTT, Dr. K. A. MCCULLY, Dr. W. P. COCHRANE, Mr. R. BLINN and Mr. J. BURKE, was provided with the 1968 IUPAC report on this subject. They were also informed that:

'For a few years the Pesticides Section of IUPAC has been giving consideration to methods of analysis for pesticide residues. One of the purposes for that consideration is in response to requests from a FAO Working Party on Pesticide Residues. The latter group has been asked to review pertinent data and propose tolerance values for residues of pesticides that may be in food products, particularly those present

during the time of international commerce. It has been agreed that when tolerances are recommended it is necessary that a method of analysis to enforce that tolerance be designated. It has also been agreed that, generally speaking, the only practical way by which residues in food of unknown pesticide treatment history can be effectively analyzed for whatever residue may be present is by use of multiresidue methods—that is, those by which a number of compounds are identified and measured simultaneously. It was also agreed that the Pesticides Section could make a valuable contribution to organizations desiring to make food analyses (such as the request from FAO) by fully investigating some of these techniques and adopting one or more of the most widely applicable methods with a view to providing it as a recommended method. It was further felt that when such methods were adopted the Section would encourage research to simplify them and to provide compatible means of easily identifying the residue so they would have wider utility.

It is recognized that the nature of this modern methodology is such that a method is “never finished” and any adoption by any organization must provide for significant improvements, additions, and extension to other chemicals. Nevertheless, they can be defined at any given time so that they provide the best possible methodology.’

The request to the Working Party further stated:

‘It is hoped that the originator of each method will assemble the pertinent supporting data available, either published or unpublished, which can be used by the Working Party and Section to support a recommendation. We would like to see the data which show the number and type of food products for which the method has been proven useful, the pesticide chemicals and their metabolic products which are quantitatively extracted and cleaned-up, and the percent recovery of each. Most of the recovery data will be from spiked samples; however, any data that are available which show the recovery of field-incurred residues would be very useful. The data to support the particular extraction system and the desirable features and performance standards of the GLC system are very important. Any confirmatory tests or other techniques by which the identity of the residues is made more certain would be useful.’

As a result of the deliberations of this Working Party, particularly stemming from the comments of Mr. BURKE (to be submitted for publication in *Pesticide Reviews*), Dr. McCULLY and Dr. COCHRANE, the list of recommendations quoted in the minutes of the Fourth Meeting of the Commission was devised.

#### *APPENDIX II: Multiresidue Methods of Analysis for Organophosphorus Compounds*

At the Third (1968) Meeting of the IUPAC Commission on Pesticide Residue Analysis it was agreed that consideration be given to multiresidue systems of analysis for the organophosphorus compounds. Each member of the Working Party developed for the organochlorine multiresidue methods (Appendix I) was asked to consider multiresidue methods for organophosphorus pesticides; later, Mr. R. W. STORHERR was asked to join the group.

Considerable work has been done in a number of laboratories on developing complete methods of analysis for residues of organophosphorus pesticide chemicals, but the work so far has not been as fruitful as the work on the organochlorine compounds. The organochlorine compounds are generally highly nonpolar compounds; thus, they are relatively easy to extract from



and clean-up in presence of polar compounds. In contrast to the organochlorine compounds, the organophosphorus ones have a wide range of polarities from those which are highly oil soluble to those which are highly water soluble. Many of those which are highly oil soluble when applied are either oxidized, isomerized, or otherwise altered to moderately or highly water-soluble, toxic residues. Techniques have been devised for extraction of both highly oil-soluble and water-soluble ones by means of acetonitrile, dimethylformamide, *etc.*; gas chromatography has been accomplished which accommodates the extremes of polarities—usually by at least 2 columns—and highly sensitive detectors have been developed. However, the clean-up step has been difficult to develop.

The *Analytical Methods for Pesticide Residues in Foods* of the Canadian Food and Drug Directorate<sup>1</sup> contains portions of procedures for a number of organophosphorus compounds. The system for organophosphates is to extract with acetonitrile. The acetonitrile is evaporated and the remaining aqueous portion is extracted with hexane. The acetonitrile extracts the polar and nonpolar residues. The hexane removes the nonpolar ones from the aqueous residue and the polar ones remain. The aqueous phase is then extracted with chloroform, which should extract the polar compounds. However, when the Manual was prepared only paraoxon had been utilized to evaluate this portion of the procedure. Gas chromatography should be no problem. We hope that at a later date more data will be available to the Working Party on this phase of the procedure.

The Laboratory of the Government Chemist in England has done considerable work on methods for organophosphorus compounds. Dr. ABBOTT supplied a recent general method<sup>2</sup> for the determination of organophosphorus pesticide residues in river waters and effluents by gas, thin-layer and gel chromatography. This general method appears to be very promising for residues of organophosphorus compounds in water. From 71 to 92% recovery was achieved for 7 compounds. A part of the procedure, that of gel separation, appears to be very promising as another parameter for confirmation of residues. The extracted pesticides are added to and then eluted from a column made from Sephadex IH20 gel beads. Different pesticides are eluted in three different fractions under controlled conditions. This technique should be equally useful in food-product residue analysis when fully developed.

Dr. ABBOTT submitted a prepublication manuscript<sup>3</sup> of the methods used in total diet analysis for residues of the parent compounds or their immediate metabolites or breakdown products of 40 organophosphorus pesticides. Cereals are extracted with methanol in a Soxhlet apparatus, the extract concentrated, put onto a charcoal column, and the residues eluted with acetone. Meats and fish, fruits and preserves, and root and green vegetables, are dried with anhydrous sodium sulphate and extracted with acetonitrile. The acetonitrile is diluted with 2.5% sodium sulphate solution and extracted with chloroform. This is dried and evaporated to dryness and the residue dissolved in acetone.

Fats are mixed with anhydrous sodium sulphate, and the mixture is extracted with hexane and then with acetonitrile. The two extracts are mixed well and allowed to separate. Then the acetonitrile portion is diluted with 2.5% sodium sulphate solution and the mixture is extracted with dichloromethane. This extract is evaporated; the residue is dissolved in acetone. Milk was mixed with anhydrous sodium sulphate and extracted with acetonitrile. The acetonitrile extract was treated in the same manner as in the procedure for the fat group.

Aliquots of the acetone solutions were utilized for total phosphorus analysis or gas-liquid chromatography on two types of column. The sensitivity

to most of the organophosphorus compounds was of the order of 1  $\mu$ g. The recovery of the compounds through the procedures was better than 70% in all cases and well in excess of this for many of the compounds concerned. This procedure was applied to 66 total diet samples. It is one of the first applications of a comprehensive multiresidue scheme for organophosphorus pesticide residue analysis.

Mr. BLINN submitted considerable information on multiresidue procedures for organophosphorus pesticides. Basically he proposed a procedure in which he combined what he considered to be the best portion of each of several previously published methods. He pointed out that 'the organophosphorus pesticide residues present unique difficulties compared to their organochlorine counterparts because of (a) the prevalence of metabolic products of toxicological interest, and (b) the wide range of polarities and chemical stabilities encountered'. Because of the above problems, he suggests that 'the multiresidue procedure should therefore include if possible a conversion of at least a portion of a pesticide's metabolites into one derivative, thereby reducing the number of residual entities required to respond to the analytical method, and as an aid to identification'. He points out that 'it is essential for the method to respond to those metabolic products of interest, because response by only the parent organophosphorus pesticides is often meaningless since hazardous metabolites may be the only survivors of the residual climate'. The method on which he based his recommendation is that of THORNTON and ANDERSON<sup>4</sup> which was designed primarily for disulfoton. He suggested an extraction procedure based on that of BOWMAN, BEROZA and LEUCK<sup>5</sup> and a hexane-acetonitrile partitioning. Then, following evaporation of the acetonitrile, a separation of the residues between water and hexane, then removing the residues in the water phase by chloroform. The residues in the hexane are adsorbed onto Nuchar and eluted with chloroform. This effects a separation of the polar from the nonpolar compounds. He then suggests oxidation of residues by the THORNTON and ANDERSON<sup>4</sup> technique followed by gas chromatography. He states that the gas chromatographic conditions of WATTS and STORHERR<sup>6</sup>; RUZICKA, THOMSON and WHEELS<sup>7</sup>; WESSEL<sup>8</sup>; or BEROZA, BOWMAN and LEUCK<sup>5</sup> would be satisfactory. He proposed that thin-layer chromatography confirmation be based on the techniques of GARDNER<sup>9</sup> and GETZ and WHEELER<sup>10</sup>.

STORHERR and WATTS prepared a review of the FDA research on the development of schemes for organophosphorus pesticides and their significant metabolic or alteration products. This review shows the results of a large amount of effort and very significant accomplishments. They reviewed and evaluated the following methods:

1. Mills procedure for non-fatty foods (the FDA-PAM—see p. 196—method recommended for organochlorine multiresidues).
2. Ethyl acetate extraction and sweep codistillation clean-up procedure for non-fatty foods<sup>11</sup>.
3. Ethyl acetate extraction and charcoal column clean-up for non-fatty foods<sup>12</sup>.
4. Acetonitrile extract aliquot and charcoal clean-up procedure for non-fatty foods.

It can be seen that the development of multiresidue methods for organophosphorus compounds and their metabolites has been actively pursued and that much progress has been made. No method has progressed to the point where we can make a recommendation with the degree of confidence that we can in the case of the organochlorine compounds. Arising from this report, the recommendations listed in the minutes of the Fourth Meeting of the Commission were proposed.

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## APPENDIX III: Fumigant Residue Analysis

**Multiresidue Methods.** HEUSER and SCUDAMORE<sup>1</sup> have completed the development and testing of a multidetection scheme for the determination of volatile residues resulting from the use of any of some 17 fumigants. The use of one polar and one nonpolar column and of two solvent systems has been standardized and the most satisfactory combinations of column and radio-active ionization detector, with its appropriate carrier gas, have been paired. A flame ionization detector is operated in series with each of these other detectors and two different solvent extracts are run on each column as necessary. In this way each of the compounds of interest can be determined with high sensitivity by one or more of the detectors without solvent interference and with some confirmation of identity, although some compromise from optimum conditions for examination of each compound must be accepted.

The scheme in outline is as follows:—

Solvent	Extract 1 5:1 v/v acetone:water	Extract 2 5:1 v/v acetonitrile:water
Column	10% w/w Carbowax 1540 on Teflon 6	Porapak Q 50-80 mesh
Carrier gas	Nitrogen	Argon
Detector (a)	Electron capture	$\beta$ -ionization
Detector (b)	Flame ionization	Flame ionization



To use the  $\beta$ -ionization detector satisfactorily, it is necessary first to remove water from the extraction solvent. The compounds tested in this detection scheme were acrylonitrile, carbon disulphide, carbon tetrachloride, chlorobromomethane, chloroform, chloropicrin, dichloromethane, dichloropropane, dimethyl sulphide, ethylene chlorohydrin, ethylene dibromide, ethylene dichloride, ethylene oxide, ethylidene chloride, hydrogen cyanide, methyl bromide, perchlorethylene, propylene oxide, and trichlorethylene. In addition, phosphine was tested, but only by injection of air samples.

Residue determinations of methyl bromide and ethylene oxide have confirmed the wide application of the solvent extraction method for these fumigants and the quantitative reliability of the methods on which the multidetection scheme is based; the initial programme on methyl bromide has been concluded<sup>2</sup>. Residual methyl bromide was satisfactorily determined in fumigated samples of wheat, wheat flour, maize, sultanas, groundnuts, groundnut and cottonseed cakes, and cocoa beans. The effect of extracting at low temperature (0° to 2°) to inhibit breakdown of methyl bromide during recovery was investigated. A similar programme of work on residues of ethylene oxide and ethylene chlorohydrin in foodstuffs fumigated with ethylene oxide is in progress. An observation of particular interest is the formation of ethylene bromohydrin in foodstuffs containing bromide, including that formed as a result of prior fumigation with methyl bromide. Under the conditions standardized for determination of the chlorohydrin (elution time 8 min) the bromohydrin peak appears after 16 min.

BEN-YEHOSHUA and KRINSKY<sup>3</sup> have briefly reported on gas chromatographic determinations of trace levels of ethylene oxide, ethylene glycol, diethylene glycol, and ethylene chlorohydrin in acetone extracts of treated date fruit using three columns with two detectors. Columns of Porapak R and of polypropylene glycol on Chromosorb W with a flame ionization detector permitted the determination of less than 1 ppm of each of these materials. With a thermal conductivity detector used in conjunction with a silanized Gaschrom P column, ethylene oxide could not be separated from acetone without temperature programming. PAGINGTON<sup>4</sup> has described the use of an Ozatron type J detector element from an AEI leak detector type HA for the determination of chlorohydrins in aqueous or solvent extracts injected directly on to a Porapak column.

*Determination of Residual Phosphine.* Although a number of workers have reported the use of GLC methods for the determination of phosphine in air, there appears to be grave difficulty in adapting these techniques to the reliable quantitative determination of small residues of phosphine in foodstuffs. DUMAS<sup>5</sup> used a thermistor thermal conductivity detector with a column consisting of Apiezon L on firebrick to determine concentrations in air from 10 mg of PH<sub>3</sub> per litre to something less than 0.5 mg per litre. BERCK<sup>6</sup> used a thermal conductivity detector with a column packed with 10% SE=30 on a silanized solid support (Diatoport S). Samples of PH<sub>3</sub> dissolved in 1-butanol were injected. The air peak was not separated from the PH<sub>3</sub> peak but it was stated that the peak area was small and constant and could be allowed for.

WAINMAN *et al.*<sup>7,8</sup> obtained good separation from air and carbon dioxide on a Porapak Q column but concluded that neither a micro cross-section detector nor a micro-katharometer detector was sufficiently sensitive. The flame ionization detector was sufficiently sensitive only for the higher range of concentration and behaved erratically from time to time. The phosphorus detector (with caesium bromide tip) proved highly sensitive to phosphine but the response was linear only over a very limited range, making sampling and

calibration procedures very difficult. Currently a  $\beta$ -ionization detector is being used for the determination of the concentrations normally encountered in fumigation work. Response appears to vary from day to day, requiring frequent calibration which is facilitated by the use of *standard* mixtures of phosphine in argon, now commercially available in cylinders. These mixtures require periodic checking by chemical methods.

BERCK, WESTLAKE and GUNTHER<sup>9</sup> have recently investigated three sensitive detectors for the determination of  $\text{PH}_3$  by GLC. A microcoulometric detector was tested by injection of  $\text{PH}_3\text{-N}_2$  mixtures directly into the cell with  $\text{N}_2$  as carrier gas and it was concluded that amounts of  $\text{PH}_3$  in the range 5 to 500 mg could be satisfactorily measured. A thermionic detector (with caesium bromide tip) used with a 4.5% fluorosilicone oil (QF1) on Chromosorb G column was found to be much more sensitive to  $\text{PH}_3$  but these workers also report that the response is nonlinear. The best results and the greatest sensitivity (to 5 pg) were obtained by a flame photometric detector method. These methods are not applied to the determination of residues.

HEUSER and SCUDAMORE<sup>1</sup> concluded that  $\text{PH}_3$  could not be included in their proposed multidetection scheme because of the difficulty of holding it in a nonreactive solvent at atmospheric pressure. In fact, in all accounts published to date of work on residues from the use of phosphine fumigants, whether of adsorbed  $\text{PH}_3$  *per se* or of undecomposed aluminium phosphide, dry and wet aeration of samples has been used with absorption of evolved  $\text{PH}_3$  in reaction mixtures for chemical analysis<sup>10-12</sup>. Further investigations of the validity and accuracy of these methods appears to be required to resolve the conflicting experimental evidence on the question of chemisorption of phosphine by foodstuffs.

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## APPENDIX IV: Organomercury Residue Analysis

During the last two years an increasing number of indications of the existence of mechanisms in nature by which inorganic mercury is converted into organomercury compounds have been reported. According to the few reports yet published<sup>1-4</sup> the conversions result in alkyl mercury compounds, especially monomethyl derivatives, and the very volatile compound dimethyl mercury. It is believed that certain types of organomercurials, *e.g.*, phenyl mercury

compounds, are decomposed into inorganic mercury before being converted into methyl mercury compounds. It seems likely that monomethyl mercury compounds are the main conversion products, and that sulphur is firmly bound to the other valency of the mercury atom although the chemical nature of the organo sulphur group is unknown. The existence of two types of methyl mercury compounds, one of them more toxic than the other, has recently been postulated but laboratory evidence is somewhat scanty.

*Analytical Methods.* Methods of analysis for residues of mercury have been reviewed by SMART<sup>5</sup>. Most of the residue analyses referred to in the previous report<sup>6</sup> were performed by neutron activation techniques (NAA). The two methods most commonly used are those of SJÖSTRAND and WESTERMARK<sup>7,8</sup> and of KIM and SILVERMAN<sup>9</sup>. Using chemical methods of purification of the irradiated sample, e.g., electrolysis on gold, sensitivities of the order of 1 ng of Hg/g are reached. Later publications do not usually claim higher sensitivities, but KOSTA and BYRNE<sup>10</sup> have also obtained this range of sensitivity by collecting the vapours of mercury in a selenium-containing filter, after combustion of the biological sample, and activating in a neutron flux.

RUZICKA and LAMM<sup>11</sup> have reported the successful use of isotope dilution methods to determine the total amount of mercury in biological samples. Using a commercial instrument for handling the solutions prepared from the samples (e.g., ignited or/and dissolved) they claim to be able to analyse a very large number of samples per day (20/hr), thus meeting the demands of rapid and inexpensive analysis when monitoring the environment. The method allows detection of less than 1 ng of Hg/g.

Although vapours of mercury are most sensitively detected by spectrophotometric methods, especially in the form of atomic absorption, only a few recent publications report the use of this method in environmental studies. However, LIDUMS and ULFVARSON<sup>12</sup> have reached sensitivities of 1 ng of Hg/g when utilizing gold traps to collect mercury liberated by combustion of biological samples. In a series of determinations, results obtained were in close agreement with those of the NAA method.

A considerable amount of work has been performed by WESTÖÖ<sup>13-16</sup> to improve gas chromatographic methods of determining organomercurials in food. The sensitivity is now better than 1 ng of Hg/g for methyl mercury using electron capture detectors. WESTÖÖ<sup>3</sup> refers to the use of mass spectrometry to prove the presence of methyl mercury contamination in some foods, the limit of sensitivity being 100 ng of Hg/g. Although a large number of gas chromatographic studies on organomercury contamination are known to have been performed in Japan, linguistic difficulties preclude reference to more than one work<sup>17</sup>. Thin-layer chromatography has been used as an effective way of cleaning up biological samples before the final quantitative analyses carried out by other methods.

During the last two years, programmes have been set up to compare the analytical results obtained in mercury analysis of biological samples. On the whole, acceptable results were obtained in the two programmes referred to<sup>18,19</sup>. Too few programmes, however, have considered the use of more than one analytical method, and as expected, the programme<sup>19</sup> dealing with several methods showed the widest deviation—about 20%. On the other hand, even this result was less disappointing than those shown in some other analytical programmes.

*Conclusions.* The following types of analytical method are those most frequently used for high-sensitivity analysis of mercury residues:



Neutron activation analysis  
Isotope dilution analysis  
Atomic absorption analysis  
Gas chromatography  
Mass spectrometry

In their appropriate forms all these methods nowadays allow determinations down to the range of ng of Hg/g sample. This degree of sensitivity seems to be sufficient for most types of biological study. However, in only a few biological studies is it enough to use one single analytical method without frequent checks against some of the other methods.

It is desirable that improvements be made to allow simultaneous determination of the most commonly-occurring types of organomercurial. Alkoxy and aryl mercurials seem to be the ones most difficult to determine, and, because of the weak electron affinity of dimethyl mercury, the estimation of this compound will require the use of alternative detectors. Regarding the insufficient knowledge of the forms in which alkyl mercury is bound to biological materials it is recommended that further studies be undertaken of the methods of cleaning-up the sample before the final instrumental analysis. It is also desirable to find improved analytical systems to allow further studies:

- (a) to differentiate between likely sources of the mercury contamination found in some countries;
- (b) of ways by which mercury might be taken out of biological circulation; this includes climatological effects;
- (c) of the different forms in which alkyl mercury is bound to the biological material, including a consideration of the so-called 'biogenic' types of organomercurial;
- (d) of other elements present in the sample which is being analysed for mercury.

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## SECTION VI.6: ORGANIC COATINGS

### 1. Meetings

The Section met on 1st and 2nd July. The following were present: FINK-JENSEN, RAASCHOU NIELSEN, HAMANN, VAN LAAR, O'NEILL, OESTERLE, PAGANI (Titular Members); TOUSSAINT, WAPLER (Associate Members).

### 2. Minutes of Previous Meeting

The minutes of the meeting in Stuttgart on 30th September and 1st October, 1968, were approved by the Members without change.

### 3. Opening Address by Chairman

After citing some of the passages of Prof. KONDRATIEV's Presidential Address which were of special relevance to the Section, the Chairman gave a brief summary of the activities since the Stuttgart meeting. As far as the German translation of the publication *Hardness Testing of Organic Coatings* was concerned, no reply had been received from the Deutsche Forschungsgesellschaft für Blechbearbeitung und Oberflächenbehandlung, which had shown interest in publishing the booklet. After a brief mention of the present Section projects, the Chairman informed the Members about some discussions which he had had with Dr. FUNKE (Forschungsinstitut für Pigmente und Lacke) concerning the possible publication under the auspices of IUPAC of a series of monographs on *Progress in Surface Coatings*.

The Chairman then dealt with the structure and the activities of the Section in the future. He referred to Dr. GALLAY's Address during the Division Committee meeting the previous day and mentioned specifically that in choosing new Members, the Section should ensure that they were good scientists, that the Members were evenly distributed geographically, and that industrial people should have a higher representation than was the case today. In order to ensure the best possible new Members, contacts could be made with national bodies, such as technicians or manufacturer associations apart from the National Adhering Organizations.

### 4. Present Activities of Section

(a) *Supplementary Training*. Prof. HAMANN informed the meeting that the replies he had received to his questionnaire had been too heterogeneous to form the basis of a report, but that he would be willing to work out a short condensed version of the replies. This was agreed upon, and in addition it was decided that each Member should publish a short article on the subject, worked out by Prof. HAMANN, in one or more paint journals in his respective country. Further contacts should be made with technical people and manufacturers who knew the need for supplementary training. On the basis of the information and opinions thus obtained, national reports should be worked out.

(b) *Symposia*. It was agreed that the arrangement of symposia on narrow, well-defined subjects on a high level fell within the working programme of the Section. After an extended discussion it was decided that Prof. HAMANN would attempt to arrange a symposium on one of three proposed subjects, probably, on *Dispersitätszustand der Pigmente in Lacke* in Stuttgart in the Spring or Autumn of 1971.

(c) *Analytical Methods for Alkyd Resins*. The leader of the Working Group, Dr. O'NEILL, reported that 6 recommendations for analytical methods for alkyd resins had been finalized, and then a collaborative investigation of



gas chromatographic identification of carboxylic acids and identification and quantitative determination of polyhydric alcohols had been carried out by Members of the Section. On the basis of the completed work, revised methods would be prepared which within a few months could be circulated to the Members for approval. A suggestion by Dr. O'NEILL that the analysis of acrylic resins should be taken up as the next task for the Working Group was accepted by all Members.

(d) *Adhesion*. After an extensive discussion it was decided that a monograph on *Paint Adhesion* should be produced by the Working Group under the Chairmanship of Dr. VAN LAAR with the assistance of 4 specialists within the field of adhesion.

(e) *Information Retrieval*. The question of cooperation within the field of information retrieval is at present being dealt with by the directors of 7 European paint research institutes, and it was agreed, therefore, that any effort on the part of IUPAC should be on a more international basis. It was decided that more information was needed about the way this important question was dealt with in countries not represented at present in the Section. It was finally agreed that in order to obtain a more complete background for further discussions of the possibilities of cooperation within this field, the Members of the Section would prepare a report on the existing literature services within the organic coatings field.

(f) *Rheological Properties of Liquid Paints*. It was agreed that a report *Assessment of Application Properties of Brushing Paints*, worked out by Mr. FINK-JENSEN and Mr. RAASCHOU NIELSEN, should be published as quickly as possible. The question as to where the report had to be published must be put to *Pure and Applied Chemistry* which had first right of refusal, but it was the opinion of the Members that the publication would only reach its audience if it was published in paint journals. The opinions were expressed that there would be interest in having the report published in English, German, French, Italian, and possibly Russian journals.

### 5. Publication of a Monograph Series

During a recent conference on surface coatings in Eastbourne, Dr. FUNKE had arranged an international meeting at which several members of the Section took part in order to discuss the possible publication of a series of monographs with high-level review articles as *Progress in Surface Coatings*. The monographs, which were expected to be 30-50 pages long, were not intended to appear at regular intervals and the editing of the series should be performed by an international group of paint scientists. It was suggested in Eastbourne that the monographs might best be published somehow or other under the auspices of IUPAC. The members of the Section agreed that such a series of monographs would be very useful to the paint industry, and that cooperation with IUPAC through the Organic Coating Section would be most desirable and offer advantages to everybody, including IUPAC. It was considered essential that the monographs appear at the latest 3 months after presentation of the manuscript and that a suitable advertising effort should be exerted. The Chairman brought up the question of authors' fees, and it was considered unrealistic by several Members to imagine that the very highly qualified writers necessary would prepare the monographs without any economic compensation. Publication could take place either through IUPAC channels or through another publishing house.

It was finally agreed that the Chairman bring up the question during the second Applied Chemistry Division Committee meeting.

## **6. New Activities**

After a discussion of possible new projects for the Section it was decided that the present activities constituted a sufficient amount of work until the meeting in 1970.

## **7. Place and Date of Next Meeting**

It was decided to hold an interim meeting in 1970 in Copenhagen, preferably in connection with the *VIth Conference of the Scandinavian Federation of Paint Technologists*.

## SECTION VI.8: WATER, SEWAGE, AND INDUSTRIAL WASTES

1. The Section met on 2nd July. The following Titular Members were present: FREYSCHUSS, GÖRANSSON, CHIPPERFIELD, DALQ, PETERS, STUNDL, TESKE.
2. The main part of the meeting was devoted to questions in connection with the *Congress on Industrial Waste Water*, which was being arranged by the Section in 1970. All the more important details concerning the Congress were settled and future work on judging reports, *etc.*, was divided between the Members.
3. During the meeting the Section also discussed the suggestion from the Italian National Adhering Organization of IUPAC that Prof. PASSINO should become a Titular Member of the Section. It was concluded that there was no urgent need to increase the number of Titular Members. It was also stated that the Section was composed of persons with special competence in various industrial waste-water questions. The lack of background information on Prof. PASSINO caused the Section to postpone the question of his membership.
4. During the Conference the Section through its Chairman and Secretary had discussions with representatives from the Fermentation Industries Section (Dr. HOOGERHEIDE, Dr. LANGLYKKE, Dr. PARISI, and Prof. SUOMALAINEN) concerning future cooperation on waste-water questions in the fermentation industries. It was agreed that further contacts should be made later when more definite plans had been formulated.

## OPEN MEETING OF APPLIED CHEMISTRY DIVISION

3rd July 1969

1. The Chairman, Dr. GALLAY, opened the meeting with an historical sketch of the Applied Chemistry Division. About 40 people attended the meeting.
2. All of the Sections, except Pulp, Paper, and Board, were represented and each Chairman gave a brief account of the work of his Section or Commission. These reports were uniformly well received.
3. The Chairman spoke of the efforts of the Division to foster as much contact as possible with industry by encouraging more industrial participation in IUPAC affairs—and by sponsoring international symposia on subjects of general interest.



## **B. 1967–1971 MEMBERSHIP LISTS OF IUPAC**

Dates indicate when a person was  
first elected to his present category  
of Membership of the relevant  
IUPAC Unit

\*

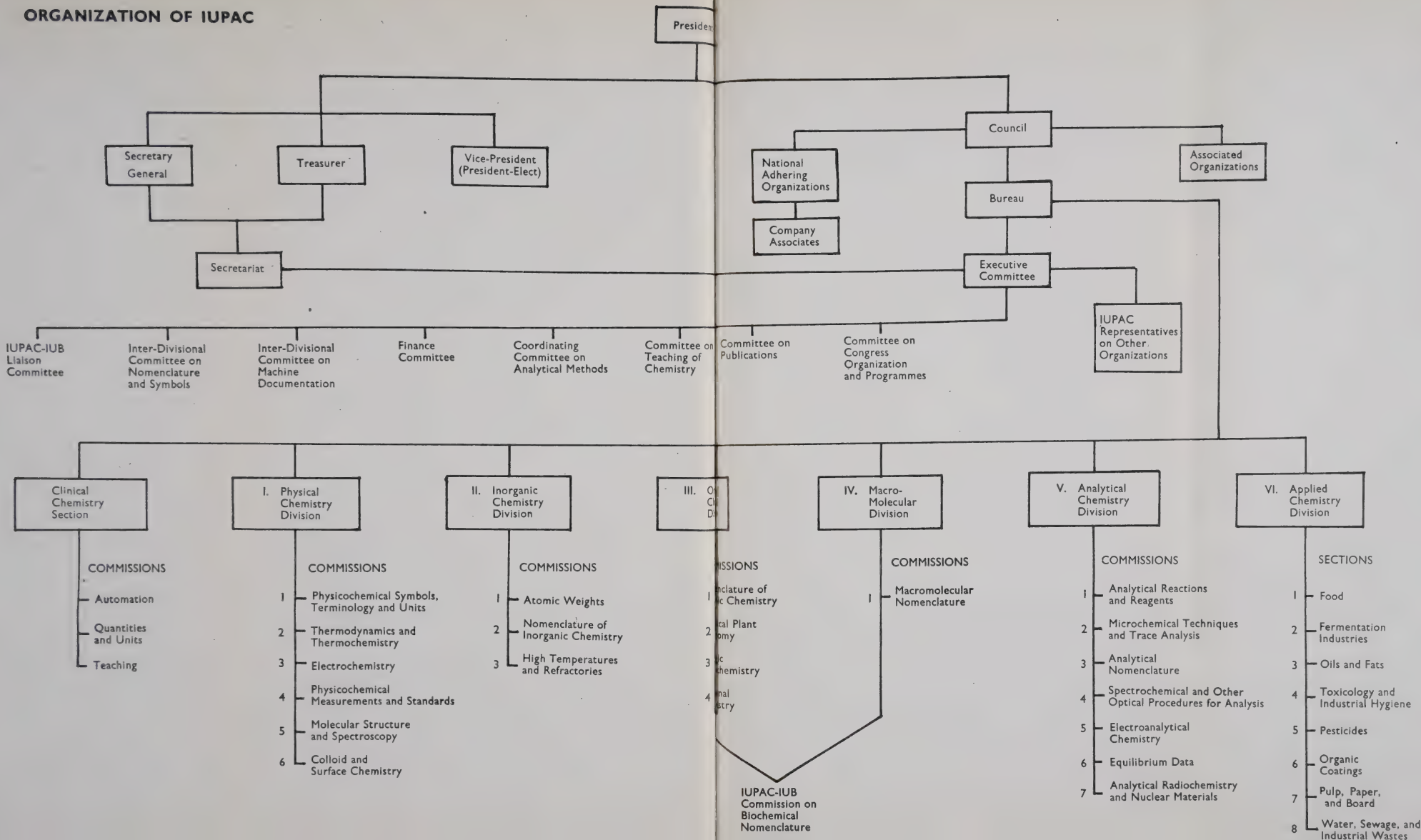
Some newly nominated Members of  
IUPAC Units are included in the  
Membership Lists subject to the  
approval of the appropriate National  
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# ORGANIZATION OF IUPAC





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- Israel* Israel Academy of Sciences and Humanities  
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Science Council of Japan, Ueno Park, Tokyo
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Postfach 1, D-8000 München 22

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### **ICSU Committee on Space Research**

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### **ICSU Scientific Committee on Water Research**

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- 1967– LORD, R. C., Prof.  
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- 1963– PLIVÁ, J., Dr.  
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- 1965– WILKINSON, G. R., Dr.  
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## **I.5.2 SUB-COMMISSION ON STORAGE AND RETRIEVAL OF SPECTROSCOPIC DATA**

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## III.2 COMMISSION ON CHEMICAL PLANT TAXONOMY

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- 1965–1973 OURISSON, G., Prof.  
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### III.3 COMMISSION ON ORGANIC PHOTOCHEMISTRY

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#### Associate Members

- 1969– GAUTIER, J. A., Prof.  
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- 1969– HUMBER, L. G., Dr.  
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- 1969– PROTIVA, M., Dr.  
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- 1969– STERNBACH, L., Dr.  
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- 1969– URBANSKI, T., Prof.  
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## IV MACROMOLECULAR DIVISION

### DIVISION COMMITTEE

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##### *President*

- 1967-1971 WICHTERLE, O., Prof.  
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##### *Vice-President*

- 1967-1971 BENOIT, H., Dr.  
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##### *Secretary*

- 1967-1971 SMETS, G., Prof.  
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- 1967-1971 BAWN, C. E. H., Prof.  
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- 1969-1971 COSSEE, P., Dr.  
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- 1968-1971 HORN, O., Prof.  
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- 1967-1971 MEDVEDEV, S. S., Prof.  
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- 1967-1971 OKAMURA, S., Prof.  
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- 1967-1971 OVERBERGER, C. G., Prof.  
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- 1967-1971 SCHULZ, G. V., Prof.  
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## Associate Members

- 1967- BUCHE, A. M., Dr.  
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- 1969- CAIRNS, R. W., Dr.  
Hercules Inc.  
Wilmington, Delaware 19899 (USA)
- 1969- KLINE, G. M., Dr.  
National Bureau of Standards  
331 South Palmway, Lake Worth, Florida 33460 (USA)
- 1967- LETORT, M., Prof.  
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- 1969- MELVILLE, Sir HARRY  
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- 1967- NATTA, G., Prof.  
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- 1967- SAKURADA, I., Prof.  
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- Australia* SOLOMON, D. H., Dr.  
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- Bulgaria* PANAYOTOV, I. M., Dr.  
1968- Institute of Organic Chemistry, Bulgarian Academy of Sciences  
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- Czechoslovakia* VESELÝ, K., Prof.  
1969- Institute of Macromolecular Chemistry  
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- Denmark* BJÖRKMAN, A., Prof.  
1968- Institute of Chemical Technology, Polyteknisk Laereanstalt  
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- Finland* SIHTOLA, H., Dr.  
1968- Finnish Pulp and Paper Research Institute  
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- France* DE VRIES, J., Dr.  
1968- Centre de Recherches de la Croix de Berny  
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- Germany* ENGEL, F., Dr.  
1968- Chemische Werke Hüls AG  
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- Hungary* TÜDÖS, F., Dr.  
1968– Central Research Institute for Chemistry, Hungarian Academy of Sciences  
Pusztaszeri út 57-69, Budapest II
- Israel* SILBERBERG, A., Prof.  
1968– Weizmann Institute of Science  
Rehovoth
- Japan* IWAKURA, Y., Prof.  
1968– Department of Synthetic Chemistry, University of Tokyo  
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- Netherlands* STAVERMAN, A. J., Prof.  
1968– Chemische Laboratoria der Rijksuniversiteit  
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- Norway* UGELSTAD, J., Prof.  
1968– Technical University of Norway, Trondheim
- Poland* TURSKA, E., Prof.  
1968– Department of Physical Chemistry of High Polymers  
Polytechnic Institute of Lodz, Zwirki 36, Lodz
- Republic of South Africa* JOUBERT, F. J., Dr.  
1968– c/o South Africa Committee for IUPAC  
South African Council for Scientific and Industrial Research  
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- Romania* SIMIONESCU, C., Prof.  
1969– Akademia Republicii Socialiste România  
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- Sweden* RÅNBY, B., Prof.  
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- United Kingdom* MELVILLE, Sir HARRY  
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- United States of America* BAILEY, W. J., Prof.  
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- 1969– SCHERAGA, H. A., Prof.  
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- 1969– WOLF, K. A., Prof.  
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## IV.1 COMMISSION ON MACROMOLECULAR NOMENCLATURE

### Titular Members

#### *Chairman*

- 1968-1971 LOENING, K. L., Dr.  
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#### *Secretary*

- 1968-1971 CROSS, L. C., Dr.  
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- 1968-1971 CORRADINI, P., Prof.  
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- 1968-1971 FOX, R. B., Dr.  
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- 1968-1971 KORSHAK, V. V., Prof.  
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- 1968-1971 SMETS, G., Prof.  
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- 1968-1971 SUHR, C., Dr.  
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- 1968-1971 TSURUTA, T., Prof.  
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- 1969–1973 FISCHER, W., Prof.  
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- 1969–1973 FREISER, H., Prof.  
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## V.I COMMISSION ON ANALYTICAL REACTIONS AND REAGENTS

### Titular Members

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#### *Secretary*

- 1968–1971 ZÝKA, J., Prof.  
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#### *Members*

- 1969–1973 HULANICKI, A., Dr.  
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- 1968–1971 KIENITZ, H., Prof.  
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- 1968–1971 PELLERIN, F., Prof.  
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- 1969–1973 REIDINGER, F. J., Mr.  
Analytical Chemistry Group, Research and Development Department, Olin Mathieson Chemical Corp.  
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- 1968–1971 SIGGIA, S., Prof.  
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- 1969– BARTOS, J., Dr.  
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- 1969– WEISZ, H., Prof.  
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## **V.2 COMMISSION ON MICROCHEMICAL TECHNIQUES AND TRACE ANALYSIS**

### **Titular Members**

#### *Chairman*

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- 1965–1973 GEL'MAN, N. E., Dr.  
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- 1967–1971 KOCH, O. G., Dr.  
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- 1965–1971 KOCH, W., Prof.  
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- 1965–1971 VEČEŘA, M., Prof.  
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### **Associate Members**

- 1969– GOMIŠČEK, S., Dr.  
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- 1965– MACDONALD, A. M. G., Dr.  
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POB 363, Birmingham 15 (UK)
- 1965– MALISSA, H., Prof.  
Institut für Analytische Chemie und Mikrochemie der Technischen Hochschule Wien  
Getreidemarkt 9, A-1060 Wien (Austria)

- 1969- MORRISON, G. H., Prof.  
Department of Chemistry, Cornell University  
Ithaca, New York 14850 (USA)
- 1969- PINTA, M., Mr.  
Services scientifiques centraux, Office de la Recherche scienti-  
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### V.3 COMMISSION ON ANALYTICAL NOMENCLATURE

#### Titular Members

##### *Chairman*

- 1965–1973 IRVING, H. M. N. H., Prof.  
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##### *Secretary*

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- 1961–1971 BAYER, E., Prof.  
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- 1969–1973 MENIS, O., Dr.  
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- 1967–1971 SAMUELSON, O., Prof.  
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- 1961–1971 SANDELL, E. B., Prof.  
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- 1969–1973 STEPHEN, W. I., Dr.  
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- 1969–1973 ZETTLER, H., Dr.  
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- 1969– ALIMARIN, I. P., Prof.  
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- 1967– AMBROSE, D., Dr.  
National Physical Laboratory, Ministry of Technology  
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- 1969– BAUDIN, G., Dr.  
Commisariat à l'Énergie atomique, Centre d'Études nucléaires  
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- 1967- BERG, E., Dr.  
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- 1969- FISCHER, W., Prof.  
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- 1967- LASTOVSKY, R. P., Prof.  
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- 1968- ROBERTSON, A. J. B., Dr.  
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- 1967- STAHL, E., Prof.  
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## **V.4 COMMISSION ON SPECTROCHEMICAL AND OTHER OPTICAL PROCEDURES FOR ANALYSES**

### **Titular Members**

#### *Chairman*

- 1957-1971 KAISER, H., Prof.  
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#### *Secretary*

- 1959-1971 FASSEL, V. A., Prof.  
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- 1967-1971 ALKEMADE, C. Th. J., Prof.  
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- 1968-1971 BILLS, K. M., Mr.  
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- 1967-1971 BIRKS, L. S., Mr.  
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- 1967-1971 KVALHEIM, A., Dr.  
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- 1969-1973 MENZIES, A. C., Dr.  
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- 1967-1971 PLŠKO, E., Dr.  
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### **Associate Members**

- 1967- DEVRIES, J. L., Dr.  
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- 1967- ROBIN, J. P., Dr.  
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- 1967- RUBEŠKA, I., Dr.  
United Nations Development Programme, Institute for Applied Research on Natural Resources  
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- 1965- STRASHEIM, A., Dr.  
National Physical Laboratory  
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1969–

WINEFORDNER, J. D., Prof.  
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## **V.5 COMMISSION ON ELECTROANALYTICAL CHEMISTRY**

### **Titular Members**

#### *Chairman*

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#### *Secretary*

- 1963–1971 ZUMAN, P., Prof.  
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#### *Members*

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- 1969–1973 GALUS, Z., Dr.  
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- 1967–1971 MEITES, L., Prof.  
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- 1967–1971 PERRIN, D. D., Dr.  
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- 1969–1973 TRÉMILLON, B., Prof.  
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- 1965– BRUCKENSTEIN, S., Prof.  
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- 1965– COETZEE, J. F., Prof.  
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Pittsburgh, Pennsylvania 15213 (USA)
- 1969– FUJINAGA, T., Prof.  
Department of Chemistry, Faculty of Science, Kyoto University  
Sakyo-ku, Kyoto (Japan)
- 1969– KAPOOR, R. C., Prof.  
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- 1969– LAITINEN, H. Prof.  
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- 1967– NÜRNBERG, H. W., Dr.  
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- 1969– VLČEK, A. A., Prof.  
Polarografický Ústav J. Heyrovského, Československá  
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### **National Representatives**

- France*  
1969– CHARLOT, G., Prof.  
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- Japan*  
1969– TANAKA, N., Prof.  
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- Poland*  
1969– KEMULA, W., Prof.  
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- United States of America*  
1969– TAYLOR, J. K., Dr.  
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## V.6 COMMISSION ON EQUILIBRIUM DATA

### Titular Members

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- 1967–1971 ANDEREGG, G., Dr.  
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- 1965– FREISER, H., Prof.  
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- 1969- LEUSSING, D. L., Prof.  
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- 1969- NANCOLLAS, G. I., Prof.  
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- 1969- PERRIN, D. D., Dr.  
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- 1969- STARÝ, J., Dr.  
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- 1969- YAMASAKI, K., Prof.  
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### **National Representatives**

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1969- Department of Inorganic Chemistry, Royal Institute of  
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- Union of Soviet Socialist Republics* YATZIMIRSKII, K. B., Prof.  
1969- Institute of General and Inorganic Chemistry, Ukranian  
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- United States of America* MARTELL, A. E., Prof.  
1969- Department of Chemistry, Texas A and M University  
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## **V.7 COMMISSION ON ANALYTICAL RADIOCHEMISTRY AND NUCLEAR MATERIALS**

### **Titular Members**

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#### *Secretary*

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- 1968-1971 HILL, K. R., Dr.  
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- 1967-1971 WIDMARK, G., Prof.  
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## **VI.5.1 COMMISSION ON TERMINAL PESTICIDE RESIDUES**

### **Titular Members**

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- 1967– KENAGA, E., Mr.  
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- 1969– KORTE, F., Prof.  
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- 1967– MOORE, J. B., Dr.  
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- 1967– POLEN, P. B., Dr.  
Velsicol Chemical Corp.  
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- 1967– PORTER, P. E., Dr.  
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- 1967– SPENCER, E. Y., Dr.  
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## **VI.5.2 COMMISSION ON PESTICIDE RESIDUE ANALYSIS**

### **Titular Members**

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- 1965–1973 RESNICK, Ch., Dr.  
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- 1967–1971 WIDMARK, G., Prof.  
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- 1967– ELGAR, K. E., Mr.  
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- 1967– KOIVISTOINEN, P. E., Dr.  
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- 1967– McCULLY, K. A., Dr.  
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- 1965-1971 FINK-JENSEN, P. H., Mr.  
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- 1967-1971 GLASER, M. A., Mr.  
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- 1967-1971 HAMANN, K., Prof.  
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- 1967-1971 VAN LAAR, J. A. W., Dr.  
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- 1965-1971 O'NEILL, L. A., Dr.  
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- 1967-1971 PAGANI, D., Prof.  
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- 1969-1973 ZVONAŘ, V., Mr.  
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- 1969- DE LA COURT, F. H., Dr.  
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- 1969- CHRISTENSEN, G., Mr.  
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- 1969- OESTERLE, K. M., Dr.  
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- 1969- RAASCHOU NIELSEN, H. K., Mr.  
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- 1967- WAPLER, D., Dr.  
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- 1969- ZORLL, U., Dr.  
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*Secretary*

- 1965–1971 SANKEY, C. A., Dr.  
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- 1967–1971 PRIOR, P. H., Mr.  
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- 1965–1971 ROGOVIN, Z. A., Prof.  
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- 1967–1971 RUTISHAUSER, M., Dr.  
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- 1969– BHARGAVA, R. L., Dr.  
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- 1967– MIGITA, N., Prof.  
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- 1965– MONZIE, P., Dr.  
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- 1967- NORIN, T., Prof.  
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- 1967- PALENIUS, I., Mr.  
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- 1967- TÖPPEL, O., Dr.  
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## **VI.8 SECTION ON WATER, SEWAGE, AND INDUSTRIAL WASTES**

### **Titular Members**

#### *Chairman*

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- 1968–1971 PETERS, H., Mr.  
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- 1968–1971 STUNDL, K., Prof.  
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- 1968–1971 TESKE, W., Prof.  
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**C. 1969 MEETINGS OF IUPAC  
UNITS OTHER THAN AT  
XXV CONFERENCE**



# COMMITTEE ON TEACHING OF CHEMISTRY

Frascati, Rome, Italy: 16-17th October 1969

## I. Attendance

The following Titular Members were present: PARRY, CHISMAN, CAMPBELL, NYHOLM, OKI, SCHWAB, SYKES. Apologies for non-attendance were received from Titular Members BÉNARD and PLATÉ. In attendance were: Prof. BAILAR (IUPAC Treasurer), Dr. W. B. COOK (ACS Division of Chemical Education), Dr. E. GIESBRECHT (Brazil), Mr. R. L. SILBER (ACS), Dr. H. TETERIN (UNESCO).

## 2. Matters Arising from Minutes of Meeting held in Oxford (12-13th April 1969)

(a) (Minute 7) *National Adhering Organizations*. The Chairman reported that a letter had been sent to all National Adhering Organizations requesting information on action taken on the recommendations of the O'CONNOR-CAMPBELL report. Replies would be collated and made available later to the Committee.

(b) (Minute 7) *Correspondent Members*. Several names of Correspondents had been suggested following the recommendation of the Oxford meeting. The following countries were involved so far: South Africa, Norway, Denmark, Hungary, Germany, Netherlands, and New Zealand. A list would be compiled as soon as the information was complete.

(c) (Minute 14) *Nomenclature*. The Chairman reported the discussions that he and the Secretary had had with Prof. MCGLASHAN during the IUPAC meeting in Cortina in July on the question of subscripts for phase in chemical equations. It was agreed not to press the suggestion of designating phase as a paranthetical subscript since the convention in the majority of books was now *on line* designation and clearly Prof. MCGLASHAN felt strongly that for the future all designations in chemical equations would be *on line*. It was agreed, however, to try to establish closer liaison with the Commission on Physicochemical Symbols, Terminology, and Units either through the Secretariat or by direct representation.

(d) (Minute 10 ii) *Next Meeting*. Dr. COOK reported that arrangements for the American Chemical Society Division of Chemical Education 50th Anniversary Meeting in Colorado were well in hand; and that it would be possible for the IUPAC Committee on Teaching of Chemistry to meet on 20th July 1970 in advance of the ACS Meeting which would be held from 21st to 25th July. Members of the IUPAC Committee would be invited to attend the ACS Meeting and to take an active part in it. The main sections of the ACS Meeting would be in Chemistry for the Citizen (non-science majors); Graduate Education of Chemistry; Chemists for the '80's; Integration of Chemistry.

The Meeting would be restricted to about 65 invited guests and the report would be available as a basis for wider discussion at the September 1970 National Meeting of ACS to be held in Chicago.

(e) (Minute 8) *Workshop on Evaluation in Chemistry*. The Secretary indicated that this report was now available—having been printed through UNESCO at the Bangkok Pilot Project—and that a bulk supply of 1,000 copies had been sent to the IUPAC Secretariat in Oxford for distribution.

It was agreed that the report should be well publicized and distributed widely. It was also agreed that a charge of \$1.50 would be reasonable in



order to offset some of the costs incurred in meeting the freightage of the bulk supply from Bangkok and distribution charges.

(f) (Minute 10 iv) *Sao Paulo Conference*. Dr. GIESBRECHT reported that the proposed conference on chemical education in Brazil had been deferred until September 1971 in view of the Colorado meeting and the ACS National Meeting in Chicago in 1970. Sponsorship of IUPAC had been requested and the necessary application forms completed.

(g) (Minute 15) *Technician Training*. Mr. SILBER reported the recent activities of ACS in technician training and in considering the professional involvement or affiliation of technicians. The US National Science Foundation had recently agreed to provide some finance towards an ACS project to develop materials for chemical-technician training courses to be tried out in a number of pilot schools over the next two years. The first writing session for these materials would be held in the summer of 1970.

The possibilities of extending this work on an international basis was discussed but the Committee agreed to reconsider the matter at the next meeting in July 1970.

(h) (Minute 10) *University Chemical Education: UNESCO Survey*. The Committee suggested the following names as authors of short articles (1,000-1,500 words) on trends in university education in chemistry:

USA:	Dr. W. KIEFFER	India:	Dr. RAMAKRISHNA (Delhi I.N.T.)
Canada:	Dr. R. J. GILLESPIE	France:	Prof. J. DUBOIS or Prof. J. BÉNARD
Israel:	Dr. D. SAMUEL	Argentina:	Prof. A. H. GUERRERO
UK:	Prof. C. EABORN	USSR:	Prof. A. F. PLATÉ
Japan:	Prof. M. OKI	Mexico:	Prof. M. MADRAZO (National Univ. Mexico City)
Brazil:	Dr. E. GIESBRECHT	Italy:	Prof. G. ILLUMINATI

Other possibilities were discussed (*e.g.*, a chemist from an African University) but it was agreed to defer further suggestions to correspondence or to the next meeting. The possibility of utilizing additional speakers at the Frascati symposium as authors of articles was mentioned.

### 3. Other Business

It was reported that Volume II of the UNESCO *New Trends in Chemistry Teaching* was now available (a few copies were distributed by Dr. TETERIN at the meeting).

Some discussion on the effectiveness of this publication took place and the Committee reaffirmed its confidence in the Editor, Mr. E. CARTMELL (University of Southampton, UK). There was, however, some concern about the high cost of the publication (42s.) and the delay in publishing. It was suggested that perhaps a small volume produced annually would be more effective. There was much sympathy with the view of UNESCO that a wider geographical coverage of authors and papers would be desirable but it was agreed that this should not be at the expense of standard of article. Reference was made to the proposed launching of an Indian Journal of Chemical Education as a possible source of articles.

It was agreed that the Secretary should discuss these views further with UNESCO and also discuss other possible areas of UNESCO collaboration with IUPAC and report to the next meeting.

#### **4. Date and Place of Next Meeting**

The next meeting would be held in Colorado, USA, on 20th July 1970.

# IUPAC-IUB COMMISSION ON BIOCHEMICAL NOMENCLATURE (CBN)

*Woods Hole, Massachusetts, USA: 4-6th September 1969*

1. The Sixth Annual Meeting of CBN since its reorganization as a Joint Commission of IUPAC and IUB was held under the Chairmanship of Prof. HOFFMANN-OSTENHOF. All Members with the exception of Dr. B. KEIL (Czechoslovakia) were present. Dr. K. L. LOENING (USA) and Prof. S. VEIBEL (Denmark) participated in the meeting as Observers for the IUPAC Commissions on Macromolecular Nomenclature and Nomenclature in Organic Chemistry (CNOC), respectively.

2. The Minutes of the 1968 meeting of CBN which had been held at Bellagio (Italy) were approved. The Chairman reported on the main activities of CBN since the last meeting. During this year three sets of tentative rules had been published in the IUPAC *Information Bulletin* as well as in several biochemical journals. These rules concern *Nomenclature of Steroids*, *Nomenclature of Cyclitols* (both prepared in collaboration with CNOC), and *One-letter Notations for Amino-acid Sequences*. They, as well as some older collections of tentative rules compiled by CBN, had also appeared in translations (French, Russian, and German).

3. A document on *Abbreviations and Symbols for Nucleic Acids, Polynucleotides, and Their Constituents* had been compiled by the Secretary with the help of several Commission Members and many specialists in the field who had been consulted. Because some American biochemists studying the physicochemical interactions of polynucleotides insisted on using symbols somewhat different from those in the document, the Chairman had invited R. L. BALDWIN, G. FELSENFELD, and H. T. MILES (all USA) as the leading representatives of this group, to join in the discussion. It was decided to make some changes and amendments to the existing document which would then be sent to the sponsoring Unions for their approval to publish it as tentative rules.

4. A document on the *Nomenclature of Vitamin B<sub>6</sub>-Compounds* which had been prepared by a CBN Sub-Commission was discussed and would be ready for publication after a few formal changes.

5. The Convenor of the CBN Sub-Commission on Polypeptide Conformation, J. KENDREW (UK), reported on the work of his group. He submitted a document which would serve as a basis for the tentative rules on *Abbreviations and Symbols for the Description of the Conformation of Polypeptide Chains*.

6. On 3rd September, the CBN Sub-Commissions on Iso-enzymes, on the Supplementation of the present Enzyme List, and on the Revision of Enzyme Nomenclature, had held a joint meeting at Yale University, New Haven. Their activities were reported and discussed. Some of the work of these Sub-Commissions was in an advanced stage and it was hoped that final drafts would soon be available.

7. A document on the *Nomenclature of Carotenoids* prepared by a Sub-Commission nominated jointly by CBN and CNOC, and already approved by CNOC at its Oberursel meeting, was examined and would now be sent to the sponsoring Unions for their approval to publish it as tentative rules.

8. A document on the *Nomenclature of Carbohydrates*, also elaborated by a Sub-Commission of CBN and CNOC, and already approved by CNOC, was examined. Because no major changes were considered necessary its

publication would be suggested. It was pointed out, however, that the present document did not cover all problems of carbohydrate nomenclature. Several nomenclature proposals, *e.g.*, for unsaturated sugars, sugar conformation, and polysaccharides, were known to have been worked out by the specialists' group. The Chairman was asked to contact the Chairman of CNOC to suggest that the existing Sub-Commission should continue its work in order to codify rules for the mentioned fields.

9. A short document on the codification and revision of the existing *Rules for the Nomenclature of Amino-acids* had been prepared by Prof. W. KLYNE (UK). This document dealt with the common amino-acids only. Prof. KLYNE and the Chairman reported on a session of the IUPAC Division of Organic Chemistry recently held in Cortina. Some members of the Division Committee had shown considerable interest in the amino-acid rules and the suggestion was made that these rules should also comprise the rarer amino-acids of which so many had now become known. It was decided to form a Sub-Commission in conjunction with CNOC to revise the present document and include the rarer amino-acids.

10. Reports on the work of the CBN Sub-Commissions dealing with (a) Nomenclature of Mucopolysaccharides, (b) Nomenclature of Tetrapyrrois and Chlorophylls, (c) Nomenclature of Non-haeme Iron Proteins, and (d) Nomenclature of Isoprenoids, were discussed. It could be expected that the activity of these Sub-Commissions would make it possible for final documents to be available at the next CBN meeting.

11. Section D of the General Rules of Nomenclature in Organic Chemistry, which would be published shortly by CNOC, included the nomenclature of organophosphorus compounds. In view of the great importance of phosphoric esters and other phosphorus compounds in biochemistry, CBN and CNOC agreed that an Appendix should be added to the phosphorus rules in Section D, indicating the particular biochemical usage in this field. A document which had been prepared by Prof. KLYNE and had been reviewed by several CBN members was discussed and amended. In its final form it would be sent to CNOC and eventually included in Section D.

12. On the afternoon of 6th September, the Commission met jointly with the IUB Commission of Editors of Biochemical Journals, to discuss matters of common interest.



## SECTION OF CLINICAL CHEMISTRY

*Geneva, Switzerland: 6th and 7th September 1969*

There was a good attendance at both meetings, 8 of the 10 Titular Members being present, as well as 11 National Representatives, 4 Observers and Dr. J. FREI as one of the representatives of the International Federation of Clinical Chemistry (IFCC) (Prof. RUBIN, one of the Titular Members, is President of IFCC). At the second meeting, representatives from Austria, Hungary, Italy, Mexico, and Poland attended, and were accepted as National Representatives from these countries for the first time.

Originally the Section was scheduled to meet at Cortina d'Ampezzo at the time of the XXVth IUPAC Conference. However, special permission was obtained from the President of IUPAC to hold the meetings in Geneva during the week before the *VIIth International Congress of Clinical Chemistry*. This change enabled many of the Section Members to attend the Congress, which proved to be a very important and worthwhile event for all of the some 1,700 clinical chemists who participated. Several of the Section Members played a vital part in the Congress. For example, Dr. SANZ, Prof. MÉTAIS, and Dr. ROTH served, respectively, as President, Vice-President, and Secretary-General of the Organizing Committee. Prof. RUBIN and Dr. FREI, as President and Secretary, respectively, of IFCC, the body which sponsors and organizes the International Congresses of Clinical Chemistry, had many duties to perform. Also, several Commission Members were involved with meetings of various Committees of IFCC. Dr. SANZ and Dr. TONKS represented the IUPAC Section of Clinical Chemistry at meetings of the Executive Council of IFCC.

The next Section Committee meeting would be held in Washington, DC at the time of the XXVIth IUPAC Conference (15-24th July, 1971). An interim meeting was being planned for the Officers of the Section in Stresa, Italy, in April 1970. The three Commissions would meet in Stresa at the same time, which would coincide with the *Italian Congress of Clinical Chemistry* (tentative dates 25th and 26th April, 1970). The three Commissions would also meet in Washington, DC at the time of the XXVIth IUPAC Conference; the Commission on Automation would hold another meeting in Birmingham, UK, in March 1971.

## COMMISSION ON AUTOMATION

*Geneva, Switzerland: 4th September 1969*

### 1. Attendance

All the Titular Members were present: SANZ, COTLOVE, JØRGENSEN, DE WAELE, WHITEHEAD.

### 2. Terminology

A proposal for terminology concerning automation, *etc.*, in analytical chemistry had been received from the Analytical Chemistry Division (Commission on Analytical Nomenclature) to be considered. This proposal was thoroughly discussed and to some extent rewritten.

### 3. Further Work on a Recommendation concerning Automated Analyses

The minutes of the previous meeting were discussed. A report, provisional for a later recommendation, was prepared.

#### 4. Future Activities

The next meeting would be in Stresa, Italy, probably towards the end of April 1970. Problems of *Safe Data Handling* and of *Monitoring Reagents* were among those to be discussed.

#### COMMISSION ON QUANTITIES AND UNITS

Geneva, Switzerland: 5th and 6th September 1969

1. The four Titular Members were all present: DYBKAER, ARMBRECHT, JØRGENSEN, MÉTAIS.

2. Members had tried to have published, reports on the IUPAC-IFCC Recommendation 1966 on quantities and units (QU-R66). More than 10 clinical chemical and clinical scientific journals had published or had accepted for publication shorter or longer versions in Danish, English, French, and German. Favourable reviews had been given to the Recommendation in several periodicals.

Many laboratories in Scandinavia and a few in USA had converted to the new system of expressing results, or were going to in 1970. The American Association of Clinical Chemists and the Scandinavian Society for Clinical Chemistry and Clinical Physiology had endorsed the principle. The journals *Clinical Chemistry* and *Scand. J. Clin. Labo. Invest.* were advocating its use by authors.

The activity report August 67-June 69 (dated 200569) was approved.

The shortened version of QU-R66 was slightly revised and would now be sent to the Section Secretary for forwarding to the IUPAC Bureau and publication.

Contact with the ISO-TC 12 Secretariat had been made and this body would consider publishing a section on quantities and units in clinical chemistry when there were a suitable number of new proposals.

3. A manuscript of 26 pages had been sent to the Members and this material was carefully examined in detail and revised. A corrected manuscript would be prepared and circulated among Commission Members.

4. Future work comprised:

(a) New proposals for quantity descriptions relevant to clinical chemistry. In the future each Member would be assigned a number of quantities for description and circulation among the other Members.

(b) Translation of a list of quantity names, sending it to all National Associations for suggestions of further inclusions, and final editing and publication.

5. The resignation of one or two Members and proposals for two or three new Members in 1971 were discussed.

#### COMMISSION ON TEACHING

Geneva, Switzerland: September 1969

The three Titular Members of the Commission were all present: RUBIN, LATNER, LOUS.

Its first project would be a review of the status of clinical chemistry throughout the world. A proposed monograph would include the history of the subject in each country, educational programmes, functions, legal status, professional and scientific organizations in the field, published journals on the subject, and the potential future development in each country. In addition to this descriptive effort the Commission had undertaken to provide recommendations for the future development of education in clinical chemistry.

To achieve this objective the Commission had enlisted the assistance of the Committee of Education of IFCC. Joint sittings with this Committee had been held in Washington, DC in 1968 and in Geneva in 1969. Through the IFCC Committee, the IUPAC Commission had now gathered some 18 reports on the subject from various countries. An additional 12 reports were expected shortly. This collection of some 30 reports from all over the world would provide the first authoritative account of the status of this important branch of pure and applied chemistry.

A complete first draft manuscript was expected before the end of 1969. After the usual clearance by proper administrative channels it was expected that publication of a final version would be completed during 1970.

The Commission had given consideration to future programmes after completion of the above work. Tentative agreement had been reached to explore the subject of the training of chemical technicians in the field, the possibility of graduate educational programmes, and the international exchange of persons for purposes of education.

## COMMISSION III.1: NOMENCLATURE OF ORGANIC CHEMISTRY

*Oberursel, Germany: 27th May-2nd June 1969*

The Commission met following a meeting of Sub-Commission II.2.1 on 25th May, 1969. The Sub-Commission had reviewed documents for Section D (coordination compounds, organometallic compounds, organophosphorus, -arsenic, -antimony and -bismuth compounds, organosilicon compounds, organoboron compounds, and chains and rings). These documents and the findings of the Sub-Commission were considered by Commission III.1 and it was decided to put these documents into the appropriate form for publication on a tentative basis by 1st October, 1969 and to distribute this new version of the rules to Members of Commissions II.2 and III.1. Comments received by 1st December would be considered for incorporation into documents to be sent to a Drafting Committee by 1st February, 1970. The resulting versions would be sent to Members of the two Commissions for approval before publication. Section D accounted for an important part of the present efforts of Commission III.1.

Documents giving rules for naming carbohydrates and carotenoids were approved with minor changes. Early publication of these documents as tentative rules was expected.

Reprinting of the *Nomenclature of Organic Chemistry*, Section A (hydrocarbons), Section B (heterocyclic systems), and Section C (characteristic groups) was planned for late 1969 with only minor revisions and extensions of subject matter. More extensive changes would be withheld until a comprehensive revision was feasible.

Prof. VERKADE announced with regret the resignation of Dr. CAHN and expressed his appreciation of Dr. CAHN's invaluable contributions to the Commission. The Chairman also mentioned his own intention to resign from the Commission in 1971 and pointed to the need of the Members to be considering a new Chairman and new Titular and/or Associate Members.

It was planned to hold the next meeting of Commission III.1 in the Netherlands from 29th August to 5th September, 1970.

## COMMISSION IV.1: MACROMOLECULAR NOMENCLATURE

*Oberursel, Germany: 3rd-7th May 1969*

The Commission considered the following major matters:

- (a) Systematic definitions of terms used in polymer science
- (b) Abbreviations and codes for common polymers
- (c) A systematic nomenclature for polymers

In all three areas drafts were prepared for further consideration and evaluation before the next meeting. A number of minor matters and correspondence were also considered.



## SECTION VI.7: PULP, PAPER, AND BOARD

Oxford, UK: 26th September 1969

### 1. Attendance

The following were present: WARD, ANKER-RASCH, SANKEY, PRIOR, RUTIS-HAUSER (Titular Members); TÖPPEL (Associate Member). Apologies for absence were received from PALENIUS and ROGOVIN.

### 2. Minutes of Prague Meeting 1967

Subject to the correction of the misspelling of the names of Dr. MONZIE and Dr. BHARGAVA, the minutes as circulated were approved.

### 3. Mechanism for obtaining IUPAC Sponsorship for Symposia

Dr. WARD drew the attention of the Section to the rules now operating for obtaining IUPAC sponsorship and subvention for symposia.

### 4. IUPAC-EUCEPA Dissolving Pulp Symposium

The symposium originally scheduled for Prague in 1968 had been cancelled due to circumstances beyond the control of the Organizing Committee. The latter had now prepared microfilms and abstracts of the papers which would have been presented (available at a cost of \$10 per set). A similar symposium on the same subject tentatively suggested for Helsinki had also been cancelled due to inadequate financial support.

### 5. Proposed Symposium in Prague

The Section agreed that it was desirable to hold a symposium in Prague, in view of the response to the cancelled meeting in 1968. Because Mr. HAVRÁNEK had been active in organizing the original symposium, the Section preferred to await proposals from him as to a suitable topic and date.

### 6. Proposed Symposium on Cellulose

The original suggestion for a symposium on this topic had been made by Prof. ROGOVIN. Since then, Prof. R. WHISTLER had approached Dr. WARD seeking the cooperation of the Section with regard to the *1972 International Conference on Carbohydrates* to be held at Madison, Wisconsin, USA. Dr. WARD thought that it should be possible to propose a full day's programme on the *Structure of Wood Carbohydrates*. Accordingly, he had written to the Organic Chemistry Division, suggesting cosponsorship of the meeting between the Pulp, Paper, and Board Section and the Organic Chemistry Division. This had met with a favourable response.

Meanwhile, the Canadian Pulp and Paper Association and the Chemical Institute of Canada had been approached re. possible cosponsorship with IUPAC and a moderate IUPAC subvention, for their joint meeting in 1972 on *Wood Chemistry*. Because no topic had yet been suggested, Dr. SANKEY was asked to convey as a possible subject *Chemical Changes occurring during Pulping* to the appropriate bodies.

### 7. 1972 Stockholm Congress on Industrial Waste Water

It was felt that the programme as outlined by the Section on Water, Sewage, and Industrial Wastes, was good. It was noted, however, that at present the

names for speakers at the section on the pulp and paper industry appeared to be incomplete. Because no reply had been received to an earlier letter on the subject, it was agreed that Mr. ANKER-RASCH should contact Dr. FREYSCHUSS to find out whether the programme had yet been finalized and whether further help was required.

Dr. TÖPPEL suggested that a section devoted to the legal requirements of this subject might be appropriate in view of its importance. Although the other Members present agreed, they felt that there would be difficulty in organizing this considering the different regulations of various countries. Nevertheless, it was felt that a useful purpose would be served if publicity was given to these differences. Therefore, it was proposed that when contacting Dr. FREYSCHUSS, Mr. ANKER-RASCH should also discuss this matter and its implications.

## **8. Proposed IUPAC-APPITA Symposium in Australia**

Reference was made to correspondence with FAO on the joint organization of a symposium on the *Pulping of Indigenous Plants*. Several Members pointed out that recently FAO and UNIDO had reorganized their projects to avoid duplication of work. At present it was not exactly clear whose responsibility various projects were, and Dr. WARD was asked to obtain clarification of the various issues when he visited Rome later this year.

It was desirable that close contact be maintained with both organizations since the Section was interested in the entire field. In particular Mr. ANKER-RASCH thought that cooperation with FAO would be useful, since at present it had little contact with the industry.

Some Members felt that *Pulping of Indigenous Plants* was too restrictive a theme because this would confine the meeting to the Eucalypts. A suggestion from Dr. PALENIUS for *Processing and Properties of High-yield Pulps* met with approval. However, Dr. BHARGAVA had, by letter, informed the Section of an International Seminar on this topic to be held in India during December 1969. Concern was felt at the lack of international publicity for this latter meeting.

In view of the desired cooperation with FAO and UNIDO, a decision on the final theme was deferred until further discussions had taken place. However, the importance of a single organizing committee in any joint venture was stressed.

## **9. Future Programme of Work**

(a) So far cooperation with the Organizing Committees of two symposia during 1972 had been discussed.

(b) Tentative proposals had been put forward for an IUPAC-EUCEPA symposium on *Man-made Polymers in Papermaking and Paper Converting* in Helsinki between 4th and 8th June, 1973. Cosponsorship by IUPAC would enable the Organizing Committee to achieve a more international meeting. It was agreed that this was desirable and that further discussions take place on the organization and programme for the meeting: Dr. WARD to act.

Mr. ANKER-RASCH expressed surprise that there was no section devoted to non-woven materials. Dr. WARD understood that this might ultimately be included. After further discussion it was suggested and agreed that this particular subject might form a theme at the XXIVth IUPAC Congress in 1973 (Hamburg). Dr. WARD would write to the German National Adhering Organization informing them of this proposal.

(c) Although symposia were extremely useful in the dissemination of information, the Members present agreed that there were several areas in the field of pulp and paper on which work was required. One of these was the analysis and testing of paper and paper products. Mr. PRIOR pointed out the need to evaluate many physical measurements. He also suggested that it was within the terms of reference of the Section to recommend analytical methods for the determination of toxic residues in the various production stages within the industry. The Section was in unanimous agreement with these proposals and requested Mr. PRIOR and Dr. RUTISHAUSER to prepare a report for the meeting in 1970, reviewing the present situation and making recommendations for a future work programme.

(d) In the past, attempts had been made to initiate a project on nomenclature. Although ISO made certain recommendations, these did not cover the entire field. Dr. TÖPPEL had prepared a short report on this subject which he presented to the meeting. In particular he stressed the need for international recommendations on symbols and terminology for dimensions used in the industry. He also suggested the need for international recommendations on the preparation of flow sheets. These proposals were accepted unanimously by the meeting and it was decided to ask Prof. CENTOLA to prepare a preliminary report by 1970 on nomenclature and abbreviations. Dr. TÖPPEL agreed to prepare a report on the action required on the question of flow sheets. In this connection he would send a questionnaire to the Head of the Pulp and Paper Institute in each country.

#### **10. Suggestions from Dr. Töppel**

Dr. TÖPPEL thought the Section should propose key words for the pulp and paper industry, for use in information retrieval. According to Dr. SANKEY, a system of English key words had already been adopted by the *Bulletin of the Institute of Paper Chemistry* (Appleton, Wisconsin) and the Canadian Pulp and Paper Institute (Montreal). It was agreed that these could possibly form the basis for further recommendations. However, in view of the recent decision by IUPAC to form an Inter-Divisional Committee on Machine Documentation in the Chemical Field, it was decided that before proceeding further, this Committee should be aware of the Section's discussions: Dr. SANKEY to act.

#### **11. Membership of Section 1969-71**

A two-year extension of term as Titular Member for Prof. ROGOVIN had been approved by the Applied Chemistry Division Committee and the Executive Committee. The nomination of Dr. R. L. BHARGAVA (India) had been approved by the Division Committee and Executive Committee and was awaiting ratification by the Indian National Adhering Organization.

#### **12. Date and Place of Next Meeting**

It was decided, subject to approval, to hold the next meeting in Stockholm at the time of the *Congress on Industrial Waste Water* in November 1970.



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## LIST OF ABBREVIATIONS

AOAC	Association of Official Analytical Chemists
AOCS	American Oil Chemists Society
APPITA	Australian Pulp and Paper Industries Technical Association
CBN	IUPAC-IUB Commission on Biochemical Nomenclature
CE	Communauté Européenne
CID	Comité International de la Detergence
CNOC	IUPAC Commission on Nomenclature of Organic Chemistry
CODATA	ICSU Committee on Data for Science and Technology
COWAR	ICSU Committee on Water Research
CREDO	Centre for Curriculum Renewal and Educational Development Overseas (UK)
EUCEPA	European Committee on Cellulose and Paper
FAO	Food and Agriculture Organization
FDA	Food and Drug Administration (USA)
IAEA	International Atomic Energy Agency
IAPT	International Association of Plant Taxonomists
IARC	International Agency for Research on Cancer
IAU	International Astronomical Union
ICC	International Congress on Catalysis
ICSU	International Council of Scientific Unions
IFCC	International Federation of Clinical Chemistry
ILO	International Labour Organization
ISO	International Organization for Standardization
IUB	International Union of Biochemistry
IUGS	International Union of Geological Sciences
IUPAB	International Union of Pure and Applied Biophysics
IUPAC	International Union of Pure and Applied Chemistry
IUPAP	International Union of Pure and Applied Physics
JCAR	ICSU Joint Commission on Applied Radioactivity
NAS	National Academy of Science (USA)
NBS	National Bureau of Standards (USA)
NCA	National Canners Association (UK)
NRC	National Research Council (USA)
OECD	Organization for Economic Cooperation and Development
OSTI	Office of Scientific and Technical Information (UK)
SAC	Society for Analytical Chemistry (UK)
SCOPE	ICSU Scientific Committee on Problems of the Environment
UICC	Union International contre le Cancer
UNESCO	United Nations Educational, Scientific and Cultural Organization
UNIDO	United Nations Industrial Development Organization
WHO	World Health Organization













